Parallel heterogeneous Branch and Bound algorithms for multi-core and multi-GPU environments

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Outline

- Context and objectives
- Contributions
 - GPU-accelerated parallel B&B Application to FSP
 - Heterogeneous B&B combining GPU and multi-core
 - HB&B@GRID: a distributed heterogeneous B&B
- Conclusions and Future Works

Exact Combinatorial Optimization



• Minimize or maximize an objective function $f(\Omega): \Omega \mapsto R$

→ Find x* ∈ Ω such that f(x*) = (min or max) f(x) / x ∈ Ω.
 → Find optimal configuration(s) among a finite set Ω of candidate solutions.

- High-dimensional and complex optimization problems exist in many areas of industry
 - Task allocation, job scheduling, network routing, cutting, packing, etc.

The permutation Flowshop Scheduling Problem (FSP)

- Scheduling a pool of N jobs on a set of M machines
 - Jobs have to be processed on the machines on the same order.
 - A machine $M_k(k = 1, 2, ..., M)$ can handle **at most one job at a time**.
- Objective

- Find a **processing order** on each M_k such that the time required to complete all jobs is **minimized**.



Optimal Solution

Branch and Bound Algorithms (B&B)

- B&B is a search algorithm based on an implicit enumeration of all candidate solutions.
- Exploration is performed by building a tree.

- Branching = splitting into sub-problems.
- Bounding = computing lower/upper bounds.
- Selection = choosing the fragment node to explore.
- **Pruning** = eliminating unpromising branches.



Illustration on FSP

- Scheduling 3 jobs on 4 machines
 3! = 6 candidate solutions
- For 50 jobs on 20 machines
 → 50! candidate solutions !!!!



- Efficient bounding is not sufficient for large instances
 - Several years of computation for Tao56 [Mezmaz et al., IPDPS 2007]

→ Massive parallelism is required to deal with very large instances.
→ All the parallelism levels provided through today's heterogeneous platforms [Top500] should be exploited

Parallel models for B&B

- Parallel B&B models [Melab 2005]
 - Multi-parametric parallel model
 - Parallel tree exploration model
 - Parallel bounding model
 - Parallel evaluation of a single solution/bound
- Parallel bounding model
 - Highly data parallel and attractive for SIMD architectures (e.g. GPU)
- Parallel tree exploration model
 - Massively parallel but highly irregular → challenging for GPU + multi-core



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Parallel Branch and Bound algorithms

- The implementation of the models is influenced by the target execution platform [Roucairol 1996, Bader 2004]
- Many architecture-oriented contributions have been proposed:
 - Networks or clusters of workstations [Quinn 1990, Tschöke 1995, Aida 2002].
 - Shared memory machines [Mans 1995, Casado 2008].
 - Graphics Processing Units [Carneiro 2011, Lalami 2012].
- Few existing works related to B&B on GPU
 → Among the two pioneering works
- No works on parallel heterogeneous (GPU + multi-core) B&B



- Revisit the design and implementation of B&B algorithms for GPUenhanced multi-core environments.
- The heterogeneous B&B should be portable in a transparent way on laptops, workstations, clusters and computational grids.
- Dealing with challenging issues related to:
 - **GPU computing:** thread divergence, hierarchical memory optimization, CPU-GPU data transfer, ...
 - •Multi-core computing: synchronization, ...
 - •Hybrid computing combining GPU and multi-core: work sharing, ...
 - •Heterogeneous cluster and grid computing: portability, scalability, ...

Contributions

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- Heterogeneous B&B combining GPU and multi-core
- HB&B@GRID: a distributed heterogeneous B&B

HB&B@GRID: A distributed heterogeneous B&B



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HB&B@GRID: A distributed

heterogeneous B&B

General GPU-based parallel model



- Data must be transferred between CPU and GPU via the PCI bus express ...
- ... many data transfers might become a
 bottleneck for performance [Mahmoudi
 2013]

Programming model: thread-based SPMD

- Kernel execution is invoked by CPU over a compute grid ...
 - ... split in a set of thread blocks
- All threads within the grid run the same program
 - Single Program Multiple Data



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- GPU architectures are based on hyper-threading
- Fast context switching ...
 - ... between warps when stalled (*e.g.* an operand is not ready)
 - ... enables to minimize stalls with little overhead
- Single instruction executed on multiple threads (SIMT) grouped into warps (32 threads)

Thread divergence issue

- If threads of a warp diverge via a datadependent conditional branch ...
 - ... the different branch paths (threads) are executed serially
- When all paths complete threads converge back to the same execution path



→Full efficiency achieved when all threads agree on their execution path

Hierarchical memory levels

Memory type	Access latency	Size
Global	Medium	Big
Registers	Very fast	Very small
Local	Medium	Medium
Shared	Fast	Small
Constant	Fast (cached)	Medium
Texture	Fast (cached)	Medium

- Different hierarchical memory levels ...

- ... with different sizes and latencies



GPU-accelerated B&B based on parallel bounding *(GB&B)*

- Bounding consumes on average 97% 99% of the B&B execution time
- Generation (selection and branching) and pruning of the subproblems ...
 - ... are performed on CPU
- Evaluation of their lower bounds ...
 - ... is executed on the **GPU** device



Thread divergence in FSP

- Lower bound proposed by [Lenstra et al. 1978] based on [Johnson 1954]
- Divergence related to the control flow instructions (*if-then-else*, *for*, ...)
 - When the first thread executes *else branch*, the remaining threads are disabled

```
if( pool[thread_idx].index_start != 0 )
   time = TimeMachines[1] ;
else
   time = TimeArrival[1] ;
```

 All threads finish the first 10 iterations together + two passes for the 90 other iterations

for(int k = 0 ; k < pool[thread_idx].index_start; k++)
jobTime = jobEnd[k] ;</pre>

Reducing thread divergence

Branch refactoring = rewrite the conditional instructions into an uniform code



I. Chakroun, M.Mezmaz, N. Melab, and A.Bendjoudi. Reducing thread divergence in a GPU-accelerated branch-and-bound algorithm. Concurrency and Computation: Practice and Experience vol 25, 8, 1121-1136, 2013 - John Wiley & Sons.

Memory access optimization

Mapping of the LB data structures on the memory hierarchy of the GPU

 Complexity analysis: The LB function uses 6 data structures with different sizes and access latencies/frequencies

Matrix	Size	Number of accesses
PTM	$n \times m$	$n' \times m \times (m-1)$
LM	$n \times \frac{m \times (m-1)}{2}$	$n' \times \frac{m \times (m-1)}{2}$
JM	$n \times \frac{m \times (m-1)}{2}$	$n \times \frac{m \times (m-1)}{2}$
RM	m	$m \times (m-1)$
QM	m	$\frac{m \times (m-1)}{2}$
MM	$m \times (m-1)$	$m \times (m-1)$

GPU memories have different sizes and access latencies



Memory access optimization (Cont.)

Memory size issue

Nvidia Tesla T10 Processor with 16 KB of shared memory

Nb.Jobs \times Nb.machines	JM	LM	PTM	RM, QM
200×20	38.000 (38KB)	38.000 (76KB)	4.000 (4KB)	20 (0.04KB)
100×20	19.000 (19KB)	19.000 (38KB)	2.000 (2 KB)	20 (0.04KB)

• JM and LM do not fit into the shared memory which size is limited

→Which data must be put in the shared memory to get the best performance?
→different explored scenarii.

N. Melab , I. Chakroun, M. Mezmaz and D. Tuyttens. A GPU-accelerated Branch-and-Bound Algorithm for the Flow-Shop Scheduling Problem. 14th IEEE International Conference on Cluster Computing, Cluster'12 (2012)".

Experimental settings

- Taillard's FSP benchmarks proposed in [Taillard 1993]
 - Optimal solutions of some of these instances are still not known
 - Divided into groups of 10 instances defined by the same N and M
 - Only the instances where M = 20 and N = 20, 50, 100, 200 are considered
 - Instances with M = 5 and 10 are easy to solve
 - Instances with 500 jobs do not fit in the memory of the GPU
- Software and hardware platforms
 - C-CUDA 4.o.
 - CPU host: Intel Xeon E5520 quad-core 64-bits server
 - GPU device = Nvidia Tesla C2050
 - 448 CUDA cores, warp size = 32, global memory = 2.8GB, configurable shared memory (16 KB or 48 KB)

Performance evaluation of GB&B

- Speedup up to **71.69** is obtained
- Speedup grows with the size of the problem
- The pool size has a high
 impact on the performance of
 GB&B



Speedups for different pool sizes

→ the pool size has to be tuned dynamically with respect to the problem being solved.

Performances evaluation of GB&B (Cont.)

Thread reduction approaches

- Best reported speedup is 77.46
- Divergent branches on average 3 times less

Data access optimization

- PTM on shared memory enhancement of 19%
- JM on shared memory acceleration of 97.83
- JM and PTM on shared memory 23% of improvement compared to the scenario with no data access optimization

→ Speedup of 100 is reached for large problem instances

Performance analysis of GB&B

Time consumption analysis of the different steps ...



→ First, the pool size should be dynamically tuned
 → Second, the CPU-GPU transfer latency should be minimized

An adaptive selection operator: Adaptive Selection Heuristic (ASH)

- Calibrates the two parameters ...
 - Maximum number of threads and blocks
- The ASH heuristic
 - The number of threads per block is **doubled repeatedly** ...
 - ... until the maximum number of active threads allowed on the device is reached
 - A downwards and an upwards search around the best pool size found so far

Algorithm 3 Template of the Adaptive Selection Heuristic (ASH).

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```
Data: nb iterations;
Result: best number of threads
max nb threads = Detect GPU Characteristics();
nb threads = Use Cuda Occupancy Calculator();
nb blocks := Get Number Of Multiprocessors();
while not empty tree() do
  while pool size \leq nb threads \times nb blocks do
     take sub problem();
  end
  Iteration pre-treatment on host side;
  Kernel evaluation on GPU;
  Iteration post-treatment on host side;
      (iteration % nb iterations = 0) and ((nb threads \times nb blocks) \leq
  if
  max nb threads) then
     if Is best pool improved() then
        best number of threads = nb threads \times nb blocks;
     end
     nb blocks := nb blocks * 2;
```

```
end
```

```
end
```



Same speedups obtained with the same best pool sizes of the static version

Performance analysis of GB&B

Time consumption analysis of the different steps ...



→ First, the pool size should be dynamically tuned
 →Second, the CPU-GPU transfer latency should be minimized

GPU-based parallel tree exploration

- Moving to GPU the branching and pruning operators
- Even if they consume less time than the bounding operator, they allow to reduce the data transfer between CPU and GPU

→ Higher performances should be achieved

- Two proposed and studied approaches
 - Multiple-nodes driven approach
 - Each thread performs in parallel B&B operators on multiple tree nodes
 - Single-node driven approach
 - Consecutive data-parallel kernels where threads compute in parallel the same amount of work on a single tree node

I. Chakroun and N. Melab. Operator-level GPU-accelerated Branch and Bound algorithms. International Conference on Computational Science, ICCS 2013. Barcelona, Spain, June 5-7, 2013.

Multiple nodes-driven approach

- Divide the search space into disjoint sub spaces
- To each thread is assigned a node from the selected nodes.
 - Mapping strategy (next slide)
- Each thread builds its local search tree by applying the branching, bounding and pruning operators to its assigned node
- Resulting nodes are moved back to CPU. Other nodes are deleted on the device memory



Multiple nodes-driven approach (Cont.)

- Mapping strategy
 - Thread i branches the node i of the pool, thread i+1 branches the nodes i+1, and so on.
 - Each thread writes the nodes it generates in an allocated range: position of thread i depends on the number of children of the thread i-1
- Challenging issues
 - Uncoalesced memory accesses
 - Thread divergence due to the high irregular nature of the tree



Example of uncoalesced access in the multiple-nodes driven approach

How much irregularity in the B&B? Intra-instance irregularity

Percentage of subproblems (%)



• At the same level (depth 10) ...

- 53% of nodes have o children, 23% have 1 child, 11% have 2 children, etc.
- At different levels
 - 41% of nodes have 17 children at depth 2 vs. 1% at depth 3

Structure of the search tree for the instance Tao23: 20 jobs on 20 machines



→ Solution: single node-driven approach

Single node-driven approach

- The same amount of work on each tree node
- Branching kernel
 - Each thread generates a unique child and inserts it into a global pool
- Bounding kernel
 - The pool is kept in the global memory and used by the bounding kernel
 - Each thread assigns a lower bound to a unique node
- Pruning kernel
 - The evaluated pool is kept in the device memory and used by the pruning kernel



Single node-driven approach (Cont.)

- Mapping strategy
 - Thread i writes the generated node i in the position i
- All threads execute exactly the same flow of instructions

Prevents from thread divergence

- The approach prevents from the uncoalesced accesses to the global memory
 - Memory accesses constitute a contiguous range of addresses.



Example of uncoalesced access in the multiple-nodes driven approach



Example of a contiguous and coalesced access in the single-node driven approach

Speedups obtained with different GPU-based approaches

- GPU-based parallel tree exploration using the single node-driven approach ...
 - ... allows further speedups (up to 160.41) than the GPUaccelerated B&B based on parallel bounding (up to 100.48).
- The single node-driven approach is more efficient than the multiple-nodes driven approach, especially for large instances.



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- Multiple-nodes driven approach
- Single-node driven approach

Speedups obtained with different GPU-based ³⁶ approaches (Cont.)

- Only the bounding operator is on GPU: GB&B
- Branching and bounding on GPU
 - From 14% to 20% of improvements compared to GB&B
- Bounding, branching and pruning on GPU
 - Further enhancement from 10% to 29%



- Multiple-nodes driven approach
- Parallel bounding
- Parallel branching and bounding
- Parallel branchning, bounding and pruning

Comparison for the different approaches in terms of data transfer

(Nb. jobs \times Nb. machines)	Bounding	Branching	Branching, Bounding
	Only	and Bounding	and Pruning
200×20	181.29 MB	180.91 MB	98.42 MB
100×20	$101.39 \mathrm{MB}$	$100.45~\mathrm{MB}$	$65.45 \mathrm{~MB}$
50×20	$1865.90 \ { m KB}$	1860.96 KB	$840.10~\mathrm{KB}$
20×20	$916.72~\mathrm{KB}$	926.26 KB	384.18 KB

- Performing branching, bounding and pruning operators on GPU reduce by 50% the average amount of exchanged data
- Low Latency GPU-accelerated B&B (LL-GB&B)
 - hides the latency induced by data transfers

→ Further transfer latency minimization by judiciously using multiple CPU cores available on nowadays resources

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HB&B@GRID: A distributed

heterogeneous B&B

ConcuRrent multi-core Low-Latency GPU-accelerated B&B (*RLL-GB&B*)

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- Challenges related to computation and data partitioning
- Concurrent GPU thread + Concurrent CPU thread
- Concurrent GPU thread
 - The idea: thread with highest priority exploits the computing power of the GPU
- Access to shared variable is handled using locks

I. Chakroun, N. Melab, M. Mezmaz and D. Tuyttens. Combining multi-core and GPU computing for solving combinatorial optimization problems. Journal of Parallel and Distributed Computing (JPDC) – Elsevier.

RLL-GB&B approach: Concurrent GPU thread

- A tree node is a leaf ...
 - the best solution is improved → updated
 - the subproblem is deleted
- Is an internal node ...
 - inserted in the pool to be off-loaded to the GPU
- Once the best pool size is reached (using ASH) ...
 - the LL-GB&B is executed



RLL-GB&B approach: Concurrent CPU thread



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Performances of the RLL-GB&B approach

- The more the number of cores is the worst the speedup is compared to LL-GB&B
- Average normalized waiting times
 - ... the GPU thread is forced to wait for the lock if it has the highest priority
 - ... waiting time increases according to the number of concurrent CPU threads



- Under-utilization of the GPU by the concurrent GPU thread
 - ➔ Cooperative approach

Idea: CPU threads prepare data for GPU using Cuda streaming + GPU (only) explores the tree

CooPerative multi-core Low Latency GPUaccelerated B&B (*PLL-GB&B*)

- Avoids synchronization issues and further minimizes the CPU-to-GPU data transfer latency
- Hides this latency by executing transfers asynchronously with kernel calls



Sequential Version



Asynchronous Versions Land 3

H2D Engine	1	2	3	4		
Kernel Engine		1	2	3	4	
D2H Engine			1	2	3	4

PLL-GB&B: Cooperative CPU thread

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PLL-GB&B: Cooperative GPU thread

- A CUDA-stream of ordered operations associated with collaborative GPU threads
- Each cooperative GPU thread handles a part of the pool of selected nodes, by performing ...
 - asynchronous transfers to the GPU device
 - calls to branching, bounding and pruning kernels
 - copies of results back to the CPU host



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Performances of the PLL-GB&B approach

- Speedups increase according to the instance size and to the number of cooperative GPU threads
- Acceleration up to 170 compared to a serial B&B
- Enhancement up to 36% compared to the LL-GB&B approach



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 - ConcuRrent multi-core Low-Latency GB&B
 - CooPerative multi-core Low Latency GB&B
 - Low Latency Multi-GPU B&B algorithm
 - HB&B@GRID: a distributed heterogeneous B&B
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HB&B@GRID: A distributed

Low Latency Multi-GPU B&B algorithm 48 (*LL-MultiGB&B*)

- The branching kernel is launched by CPU thread 1 and executed on GPU 1
 - The resulting pool is moved to the memory of GPU 2 using the peerto-peer access mechanism
- The first CPU thread prepares the pool of the next nodes to be explored
- CPU thread 2 launches the bounding and pruning kernels on GPU 2
 - Applied on the result of branching (sent by GPU 1)



Speedups using single/multiple GPUs



Speedup up to 217 with 4 GPUs for the (200 x 20) problem instances

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- HB&B@GRID: a distributed heterogeneous B&B
 - The B&B meta-algorithm
 - The B&B@Grid approach
- Conclusion and Future Works



HB&B@GRID: A distributed

A large-scale adaptive heterogeneous multicore GPU-accelerated B&B algorithm





Overall design of the adaptive heterogeneous B&B (*HB&B@GRID*)



- Combining two hierarchical levels of parallelism
 - B&B@GRID master-workers approach [Mezmaz et al., 2007]
 - ... splits the B&B tree among multiple nodes
 - B&B meta-algorithm
 - ... dynamically selects the parallel B&B to be deployed according to the underlying configuration

The B&B meta-algorithm

meta-algorithm detects The number of supplied CPU cores and **GPU devices**

- **LL-GB&B:** single CPU + single GPU
- MC-B&B: multi-core CPU without **GPUs**
- GPU
- LL-multiGB&B: multi-core CPU + multiple GPUs

Algorithm 15 Template of the proposed meta-algorithm.

max nb devices = Detect GPU Characteristics();

the max nb cores = Get CPU Characteristics();

```
if max nb devices = \theta then
  Run MCB&B algorithm();
```

end

```
else if max nb devices = 1 && max nb cores < 2 then
Run LLGB&B algorithm();
```

end

```
PLL-GB&B: multi-core CPU + single else if max_nb_devices = 1 \&\& max_nb_cores >= 2 then
                                           Run PLLGB&B algorithm();
```

```
end
```

```
else if max nb devices > 1 then
  Run LL-MultiGB&B algorithm();
```

```
end
```

The B&B@Grid approach



- The approach uses a special description ...
 - Each node is assigned a **number**
 - Work unit (collection of nodes) = an interval

- The approach is **Dispatcher-Worker** based on the **work stealing** paradigm
 - Dispatcher: maintains a pool of work units (intervals) and the global solution found so far
 - Worker: performs B&B on a given interval and updates the global solution

The HB&B@GRID approach: experimental results

- For a same computational power, the GPU-based B&B is more efficient than a distributed CPU-based B&B
- Using 3 distant GPUs is 5 times faster than 50 CPUs
- Using 5 GPU devices allows accelerations twice higher than those obtained using 500 CPU cores



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Conclusions and general insights

- GPU-accelerated parallel B&B
 - Parallel bounding on GPU using branch refactoring and shared memory allows high speedups (up to ~100 in our work) ...
 - The computation applied on tree nodes (e.g. bounding function) should be shared-data intensive and contain conditional instructions with long branches
 - ... is more efficient if combined with GPU-based tree exploration (accelerations up to ~160)
 - The overhead induced by CPU-GPU data transfer is minimized by ...
 - Auto-adapting the size of the pool off-loaded to the GPU and FSP instance to be solved
 - Limiting the **granularity** of each thread to a **single tree node**

Conclusions and general insights (Cont.)



- Heterogeneous B&B combining multi-GPU and multi-core
 - Higher speedups (up to 217 in this work) could be obtained ...
 - using the cooperative low latency data/work partitioning ...
 - ... based on the CUDA data streaming to further reduce the cost of CPU-GPU data transfer
 - ... and the **P2P memory access** between GPUs
- Large scale B&B (multi-GPU+multi-core+grid computing)
 - Heterogeneous B&B meta-algorithm + B&B@Grid
 - Auto-adaptive to the target execution hardware configuration
 - Solving very large problem instances
 - Proof of concept on (20 x 20) FSP instances (4,5h 108h)

Future work

- Extending HB&B@Grid with GPU-level check-pointing ...
 - ... for solving (50 x 20) FSP instances (years of computation!)
- Considering other ...
 - bounding functions (library): adaptive selection of bounding operator
 - exact tree-based methods (B&X), problems
 - Ph.D thesis of Rudi Leroy (Maison de la Simulation)
- Investigating other perspectives ...
 - in-house to energy-aware cloud-based HB&B
 - adapting to multi and many-core evolution with more advanced features (e.g. Kepler GPU - Nvidia GPUDirect, MIC, ...)

International Publications

International journals (3 accepted + 1 submitted)

- <u>I. Chakroun</u>, N. Melab, M. Mezmaz and D. Tuyttens. Combining multi-core and GPU computing for solving combinatorial optimization problems. Journal of Parallel and Distributed Computing (JPDC) - Elsevier.
- <u>I. Chakroun</u>, M.Mezmaz, N. Melab, and A.Bendjoudi. *Reducing thread divergence in a GPU-accelerated branch-and-bound algorithm*. Concurrency and Computation: Practice and Experience vol 25, N° 8, pages 1121-1136, 2013 John Wiley & Sons.
- N. Melab, <u>I. Chakroun</u>, and A. Bendjoudi. *GPU-accelerated Bounding for Branch-and-Bound applied to a Permutation Problem using Data Access Optimization*. Concurrency and Computation: Practice and Experience John Wiley & Sons.
- <u>I. Chakroun</u> and N. Melab. Towards an heterogeneous and adaptive parallel Branch-and-Bound algorithm. Journal of Computer and System Sciences - Elsevier (Submitted).

International conferences (4)

- Elsevier Intl. Conf. e on Computational Science (Elsevier ICCS'13)
- 14th IEEE Intl. Conf. on Cluster Computing (IEEE CLUSTER'12)
- 14th IEEE Intl. Conf. on High Performance Computing and Communications (IEEE HPCC'12)
- 9th Intl. Conf. on Parallel Processing and Applied Mathematics (LNCS, PPAM'11)

Book Chapters (1)

• <u>I. Chakroun</u> and N. Melab. *GPU-accelerated Tree-based Exact Optimization Methods Designing scientific applications on GPUs.* **CRC Press, Taylor & Francis G**roup.