Ordonnancement pour la mémoire et les transferts de données

Scheduling for memory and data transferts

Loris Marchal (CNRS & ENS de Lyon)

COMPAS 2022, Amiens.

Introduction & Motivation

- ▶ (Fast) Memory: place to store data for compute
- ► Always been a limited resource (4KB in Apollo 11 computer)
- Not limited anymore ?
 a few GB (laptops) 1TB (servers)

But problem size always gets bigger...

And this is rather a question of speed!

Annual improvements:

Time per flop (computation): 59%

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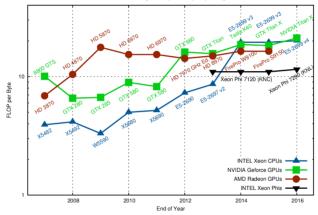
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Flop per byte moved ratio

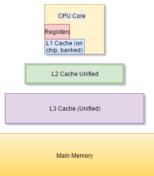


Theoretical Peak Floating Point Operations per Byte, Single Precision

ratio computing speed/communication speed From http://www.karlrupp.net/2013/06/cpu-gpu-and-mic-hardware-characte ristics-over-time/

Beyond the memory wall

- \blacktriangleright Time to move the data > Time to compute on the data
- Similar problem in microprocessor design: "memory wall"
- Traditional workaround: add a faster but smaller "cache" memory
- Now a hierarchy of caches !



Computing with bounded cache/memory

- Limited amount of fast cache
- Performance sensitive to data locality
- Optimize data reuse
- Avoid data movements between memory and cache(s) (time-consuming and energy-consuming)

In this talk: some algorithmic approaches to this problem

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Impact of Algorithm Design on Data Movements

Scheduling Task Graphs with Limited Memory

Reducing Data Movements for Independant Tasks on GPUs

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Example: matrix-matrix product

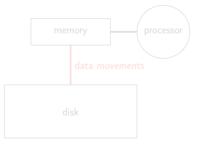
- Consider two square matrices A and B (size $n \times n$)
- Compute generalized matrix product: $C \leftarrow C + AB$

```
Simple-Matrix-Multiply(n, C, A, B)
for i = 0 \rightarrow n - 1 do
for j = 0 \rightarrow n - 1 do
for k = 0 \rightarrow n - 1 do
C_{i,j} = C_{i,j} + A_{i,k}B_{k,j}
```

Assume simple two-level memory model:

- Slow but infinite disk storage (where A and B are originally stored)
- ► Fast and limited memory (size *M*)

Objective: limit data movement between disk/memory NB: also applies to other two-level systems (memory/cache, etc



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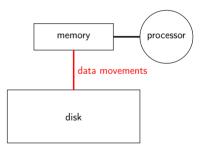
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 Question: How many data movement in this algorithm ?

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• Assume the memory cannot store half of a matrix: $M < n^2/2$

Question: How many data movement in this algorithm ?

Answer:

- \blacktriangleright all elements of *B* accessed during one iteration of the outer loop
- At most half of B stays in memory
- At least $n^2/2$ elements must be read per outer loop
- At least $n^3/2$ read for entire algorithms
- Same order of magnitude of computations: $O(n^3)$
- Very bad data reuse Question: How to do better ?

Blocked matrix-matrix product

- Divide each matrix into blocks of size $b \times b$: $A_{i,k}^{b}$ is the block of A at position (i, k)
- Perform "coarse-grain" matrix product on blocks
- Perform each block product with previous algorithms

```
Blocked-Matrix-Multiply(n,A,B,C)

b \leftarrow \sqrt{M/3}

for i = 0, \rightarrow n/b - 1 do

for j = 0, \rightarrow n/b - 1 do

for k = 0, \rightarrow n/b - 1 do

Simple-Matrix-Multiply(n, C_{i,j}^b, A_{i,k}^b, B_{k,j}^b)
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Blocked matrix-matrix product – Analysis

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Question: Number of data movements ?

- ► Iteration of inner loop: 3 blocks of size $b \times b = \sqrt{M/3}^3 = M/3$ → fits in memory
- At most M + M/3 (O(M)) data movements for each inner loop (reading/writing)
- Number of inner iterations: $(n/b)^3 = n^3/(M/3) = O(n^3/M\sqrt{M})$
- Total number of data movements: $O(n^3/\sqrt{M})$

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Question: Can we do (significantly) better ?

- Phase: consecutive subsequence of computation with exactly *M* read operations (last phase may have < *M* reads)
- Number of data available for computation in each phase:

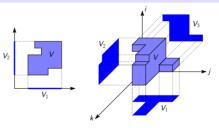
 $\leq M$ (initially in the memory) + M (read during the phase)

Crude bound on the number of elements of A, B and C used/computed: N_A ≤ 2M, N_B ≤ 2M, N_C ≤ 2M

A Helpful Geometric Lemma

Theorem (Irony, Toledo, Tiskin, 2008).

Using N_A elements of A, N_B elements of B and N_C elements of C, we can perform at most $\sqrt{N_A N_B N_C}$ distinct products.



Theorem (Discrete Loomis-Whitney Inequality).

Let V be a finite subset of \mathbb{Z}^3 and V_1, V_2, V_3 denotes the orthogonal projections of V on each coordinate planes, we have

 $|V|^2 \leq |V_1| \cdot |V_2| \cdot |V_3|,$

I/0 Bound

- Number of elementary product done in one phase: at most $\sqrt{N_A N_B N_C} \le \sqrt{(2M)^3}$
- ▶ In total: n^3 elementary products
- Number of phases: at least $\frac{n^3}{\sqrt{(2M)^3}}$ Number of reads: at least $\frac{n^3}{2\sqrt{2}\sqrt{M}}$

Theorem (refined version, Langou 2019).

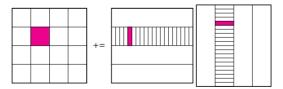
The total volume of I/Os is bounded by:

$$V_{I/O} \geq \frac{2N^3}{\sqrt{M}} + N^2 - 2M$$

Optimal algorithm

Consider the following algorithm sketch:

- Partition C into blocks of size $(\sqrt{M}-1) \times (\sqrt{M}-1)$
- Partition A into block-columns of size $(\sqrt{M} 1) \times 1$
- Partition *B* into block-rows of size $1 \times (\sqrt{M} 1)$
- For each block C_b of C:
 - Load the corresponding blocks of A and B on after the other
 - For each pair of blocks A_b, B_b , compute $C_b \leftarrow C_b + A_b B_b$
 - When all products for C_b are performed, write back C_b

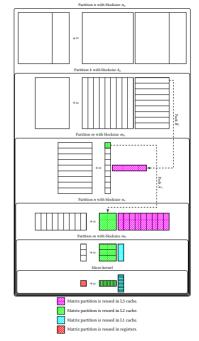


Purely theoretical algorithm?



- Introduced in the 80s as a standard for LA computations
- Written first in FORTRAN
- Library provided by the vendor to ease use of new machines
- Automatic Tuning: ATLAS
- GotoBLAS

Matrix product: still a large share of LA computations



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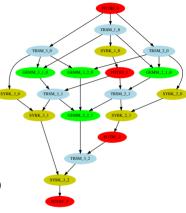
Taming HPC platforms with runtime systems

- Write you application as function calls (tasks),
- Specify data input/output (dependencies)
- Provide function codes for specific cores/GPUs
- Let the system do the scheduling at runtime!

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for(i=0; i<N; i++)
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for(k=0; k<N; k++)
MULT_ADD(C[i,j], A[i,k], B[k,j])</pre>
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Graph of tasks: Directed Acyclic Graph (DAG)

- Tasks linked with data dependency
- Wide literature on DAG scheduling
- What about memory and data movements (I/Os) ?



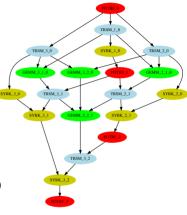
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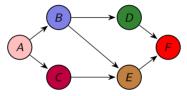
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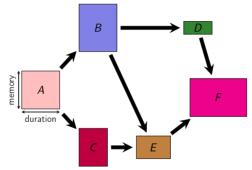


- Consider a simple task graph
- Tasks have durations and memory demands



- Peak memory: maximum memory usage
- Trade-off between peak memory and makespan

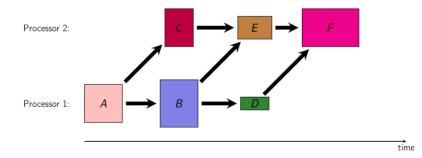
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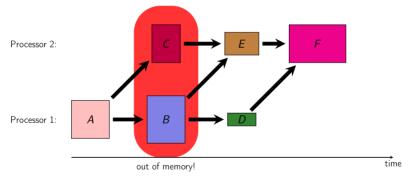
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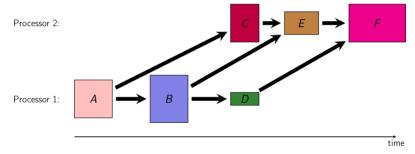
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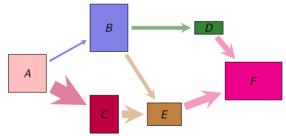
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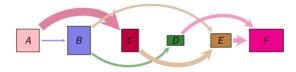
Going back to sequential processing

- Temporary data require memory
- Scheduling influences the peak memory



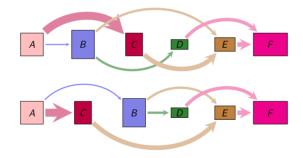
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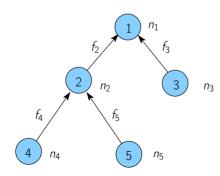
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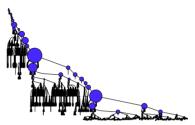
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Tree-shaped task graphs

- Multifrontal sparse matrix factorization over runtimes
- Task graph: tree (with dependencies towards the root)
- Large temporary data





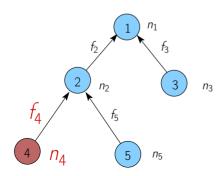
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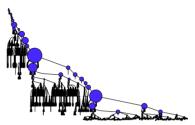
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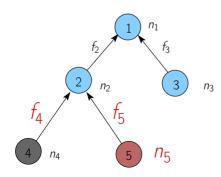


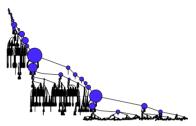
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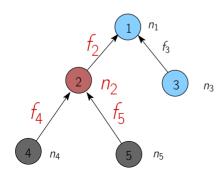
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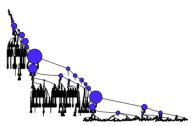
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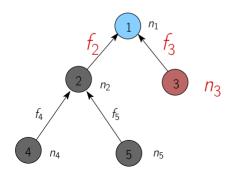
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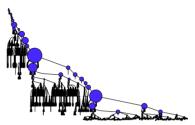
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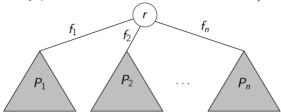


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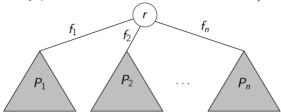
Post-Order: entirely process one subtree after the other (DFS)



For each subtree T_i: peak memory P_i, residual memory f_i
 For a given processing order 1,..., n, the peak memory is:

 $\max\{P_1, f_1 + P_2, f_1 + f_2 + P_3, \dots, \sum_{i < n} f_i + P_n, \sum_{i < n} f_i + n_r + f_r\}$

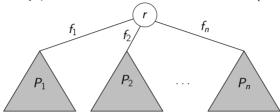
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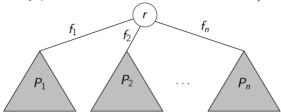
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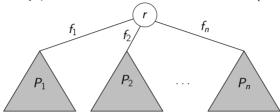
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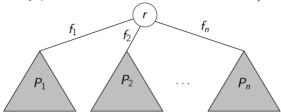
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• Optimal order: non-increasing $P_i - f_i$

Minimize the memory with single processor:

- Sest post-order schedule on trees [Liu 1986]
- Optimal schedule on trees [Liu 1987]
- ▶ ☺ Optimal schedule for Series-Parallel Graphs [Kayaaslan et al., 2018]
- ▶ ⓒ General graphs: PSPACE complete [Gilbert et al., 1980]

Parallel processing: bi-criteria problem (makespan and shared memory)

▶ ⓒ NP-complete on trees [Marchal et al., 2013]

What to do if you cannot control the schedule?

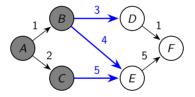
- Task graph scheduled at runtime (dynamic)
- How to make sure not to exceed available memory?



- 1. Compute worse achievable memory (topological cut with maximum weight)
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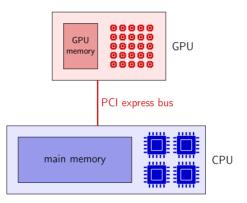
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Platform model



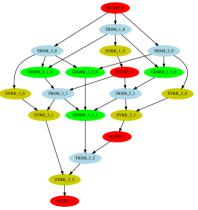
GPUs provide large speed-ups for reduced energy, but:

- limited memory within GPU
- connected through bus with limited bandwidth

Tasks available for scheduling in runtime systems

At any time step: consider only available tasks

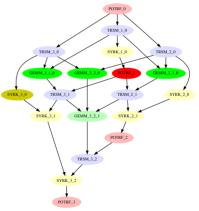
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- Sharing some input data



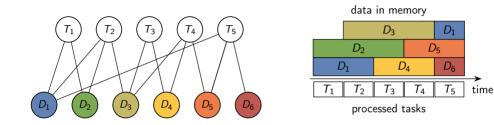
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- Sharing some input data

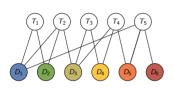


Independant tasks sharing data



- Bipartite graph modeling data sharing among tasks
- Only 3 data allowed in memory (in this example)
- Some data may be evicted/reloaded $(D_1 \text{ here})$

Problem modeling



- Bipartite graph (tasks sharing input data)
- Homogeneous data (size=1)
- Homogeneous tasks (duration=1)
- Limited memory M

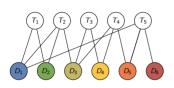
Objective: minimize data loads

Execution framework: repeat these 3 phases

- 1. Evict some data from the memory
- 2. Load some new data
- 3. Compute next task

A priori: complex description of the solution

Problem modeling



- Bipartite graph (tasks sharing input data)
- Homogeneous data (size=1)
- Homogeneous tasks (duration=1)
- Limited memory M

Objective: minimize data loads

Execution framework: repeat these 3 phases

- 1. Evict some data from the memory \rightarrow which data to evict?
- 2. Load some new data \rightarrow which data to load?
- 3. Compute next task \rightarrow which task order?

A priori: complex description of the solution

Simplifying the solution

Say we decided the task order.

Theorem (straightforward).

Thou shalt load data as late as possible.

 \Rightarrow Load (missing) data for a task right before its processing.

Theorem (adaptation of Belady's rule).

Thou shalt evict data whose next usage is the furthest in the future.

Belady's rule: optimal policy for cache management

Difference: here each task requests several data

So we only need to compute the best task order!

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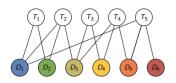
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Back to our problem



- Tasks sharing input data
- Limited memory M
- Objective: minimize data loads

Repeat:

- 1. If needed, evict data used furthest in the future
- 2. Load missing data for next task
- 3. Compute next task

Until all tasks are processed.

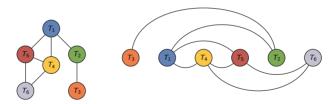
Single question: find task order

Link to cutwidth minimization

Special case:

- Each data shared by at most 2 tasks
- Objective: Load each data exactly once (never evict useful data)

Another graph model: vertices=tasks, edges=data shared among tasks



► Ordering tasks ⇔ Linear arrangement of vertices

 Amount of data in memory (maximum number of edges cut by a vertical line)

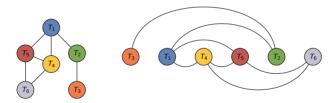
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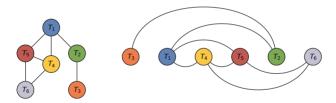
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- ► Amount of data in memory ⇔ cutwidth (maximum number of edges cut by a vertical line)

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Building packages of tasks

When the problem is too hard

Change the problem!

Build packages of tasks sharing a lot of common data

- ► All inputs within a package fit in memory
- Minimal number of packages

Then, schedule packages one after the others

Building packages of tasks

When the problem is too hard

Change the problem!

Build packages of tasks sharing a lot of common data

- ► All inputs within a package fit in memory
- Minimal number of packages

Then, schedule packages one after the others

Unfortunately, this is also an NP-complete problem 🙁

Heuristic to build packages

Hierarchical Fair Packing:

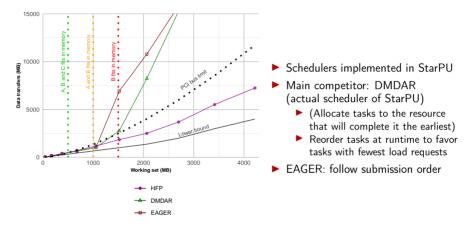
- 1. Start with each task being a package
- 2. Merge small packages sharing many input data
- 3. Stop when total input data exceed memory bound

Optimizations:



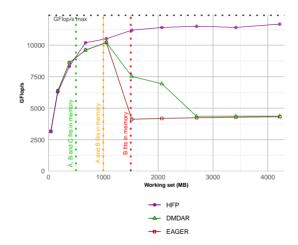
Continue merging packages when the memory bound is reached: improve locality among packages

Validation – data movements



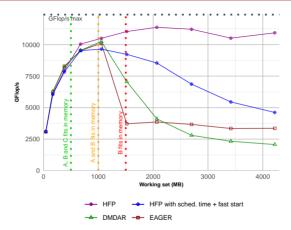
- ► 3D matrix multiplication
- Data-movements close to the lower bounds
- DMDAR leads to large data-movement as soon as memory is limited

Validation – performance in simulations



 Optimizing data movements allows to keep peak performance even when memory is limited

Validation – performance in real experiments

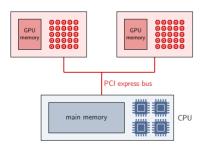


Performance very similar to simulation for small sizes

Impact of the complexity for large sizes

Shortcomings & final objective

- Large pre-computation time for large sizes (comparing and merging the packages)
- Real objective: distributed setting Several GPUs, with their own memory, sharing the bus



Two problems:

- Partition tasks among GPUs
- Order tasks within a GPU

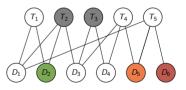
Demand-driven heuristics

Whenever a GPU requires some more work:

- ▶ Find the new data that enables the greatest number of available tasks
- Transfer this new data
- Allocate all enabled tasks to the GPU

What about eviction:

- \blacktriangleright No complete vision of the future \bigcirc
- ► Window of allocated tasks ☺
- Perform Belady's rule with this limited prediction





DARTS (Data-Aware Reactive Task Scheduling)

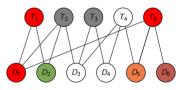
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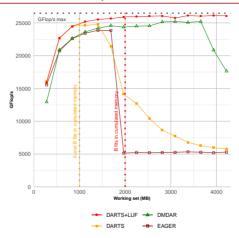
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DARTS (Data-Aware Reactive Task Scheduling)

Performance on 2 GPUs (real experiments)



- DARTS is able to achieve peak performance
- Good eviction policy is critical ! (LUF:adapted Belady's rule, otherwise:LRU)

Conclusion

Take-away messages:

- Concentrate on data movements is the key for performance
- Algorithm design can help re-organizing computations for better data reuse
- ▶ With help from: compilation, cache management,
- Runtime scheduling of task graphs: avenue for scheduling research, with specific constraints (low complexity, limited knowledge, possible pre-computation, ...)