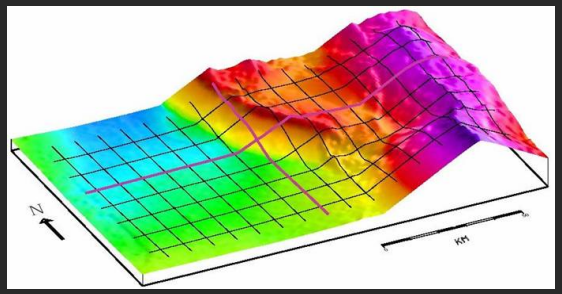
Minimisation de la mémoire VS minimisation du volume d'E/S dans les méthodes de factorisation de matrices creuses

Abdou Guermouche, LaBRI Bordeaux

May 2010

Context

Solving sparse linear systems



$$Ax = b$$

$\Rightarrow$ Direct methods: $A = LU$

Typical matrix: BRGM matrix

- 3.7×10^6 variables
- 156×10^6 non zeros in A
- 4.5×10^9 non zeros in LU
- 26.5×10^{12} flops

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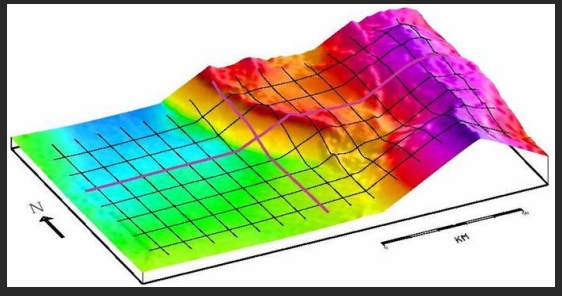

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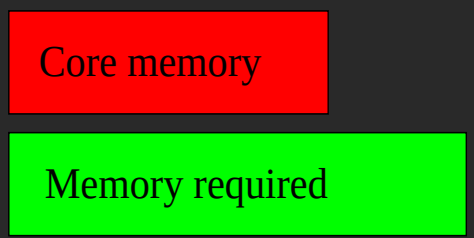
Physical constraint



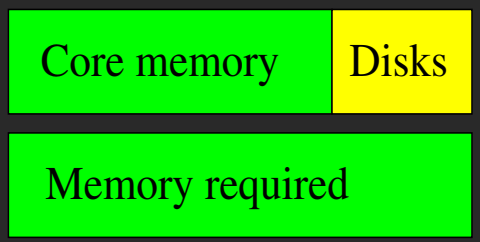
Memory crash

Software challenge

- Implementation of an out-of-core execution scheme within MUMPS

Context

Out-of-core



Use of disks

Software challenge

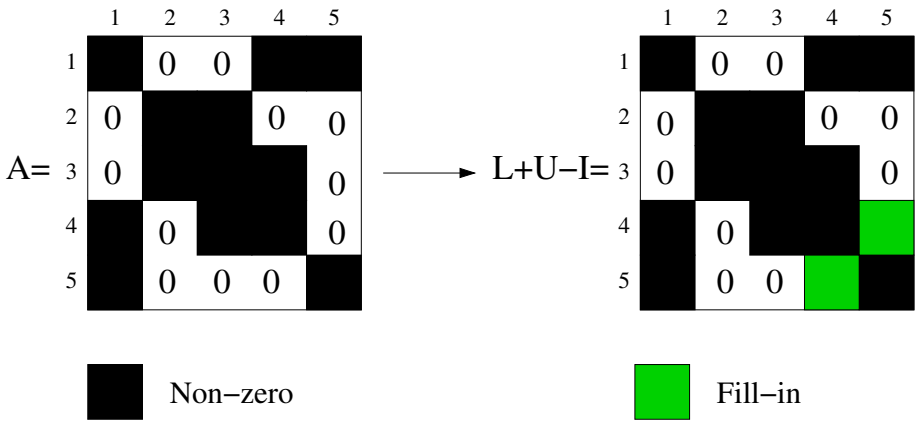
- Implementation of an out-of-core execution scheme within MUMPS

Outline

- Multifrontal method
  - Active memory minimization Algorithm (Liu's Algorithm)
- Memory issues
  - Limitation of the approach
  - New multifrontal schedules and algorithms
    - Flexible allocation scheme
    - A new memory minimization algorithm
  - Results
  - Total memory minimization
- How about Volume of I/O?
  - Computing Volume of I/O
  - Minimizing I/O volume
  - Towards an out-of-core flexible allocation
- Conclusion and Future work

Outline

The multifrontal method (Duff, Reid'83)



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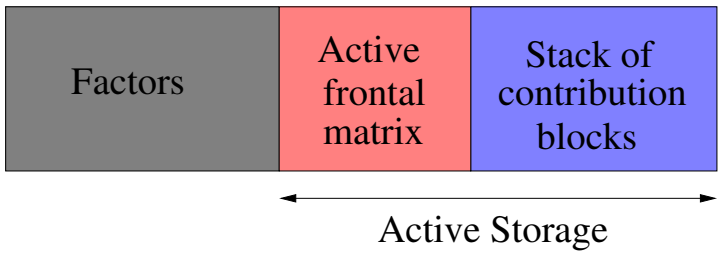

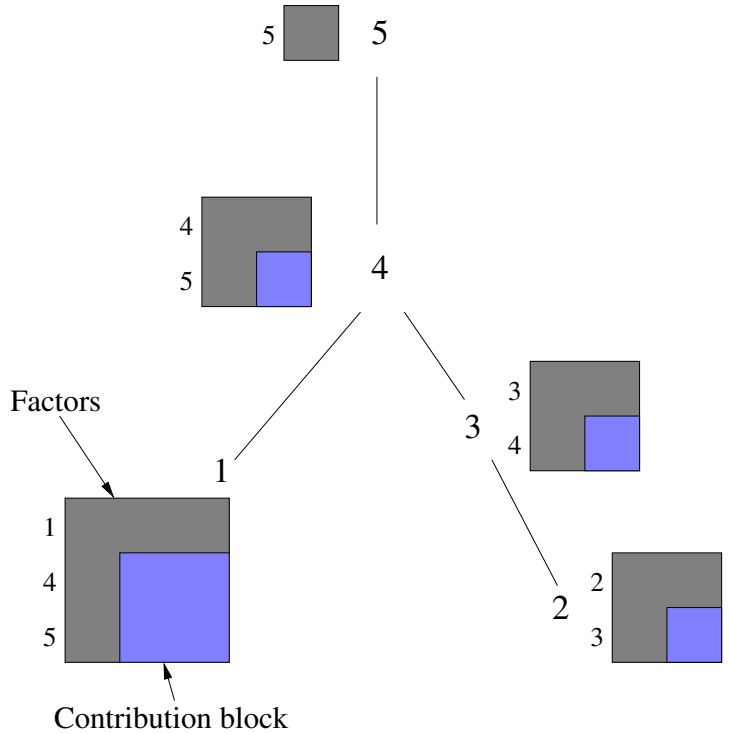

Elimination tree

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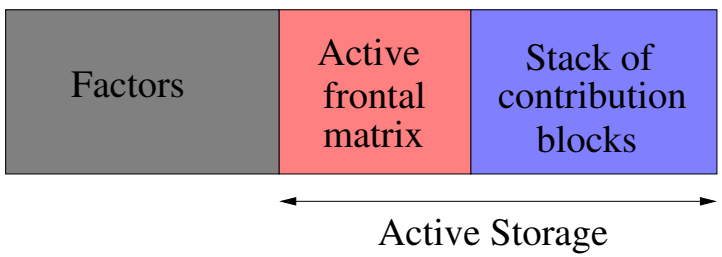

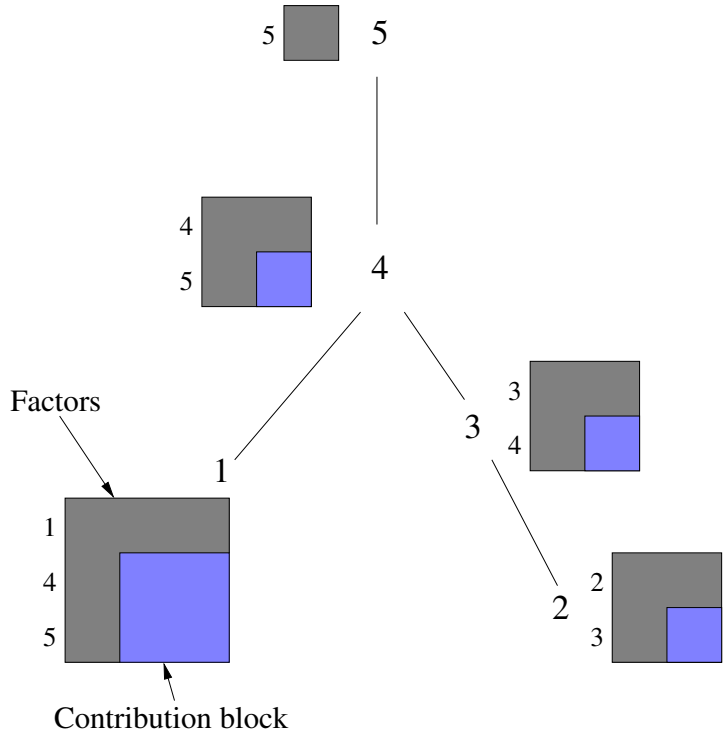

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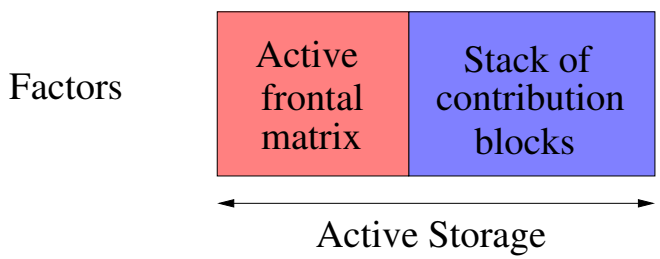

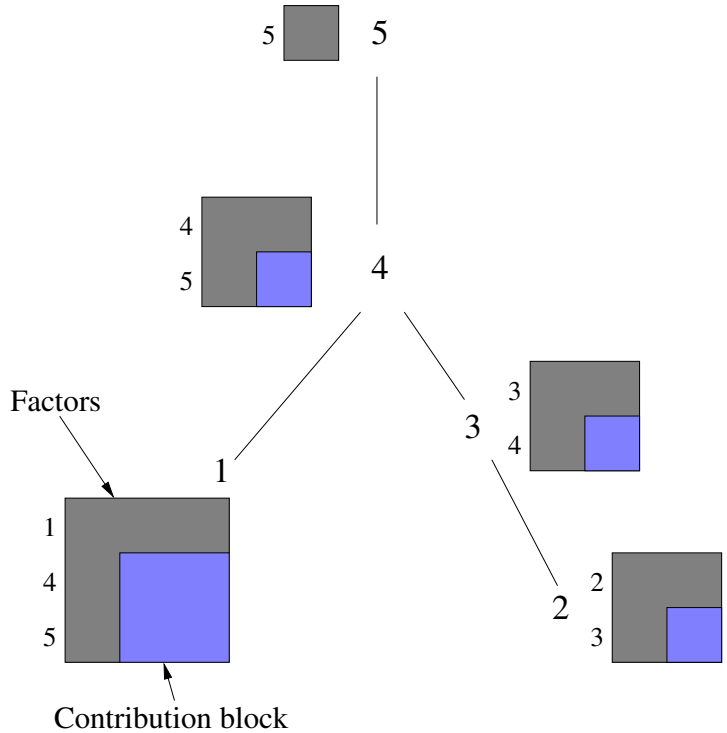

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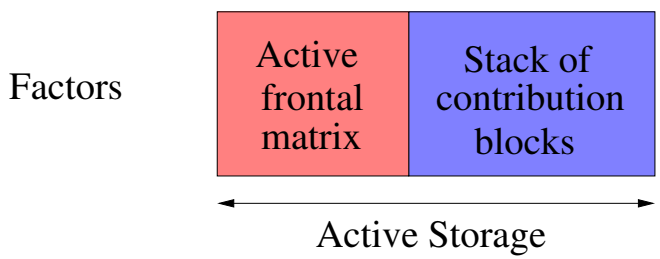

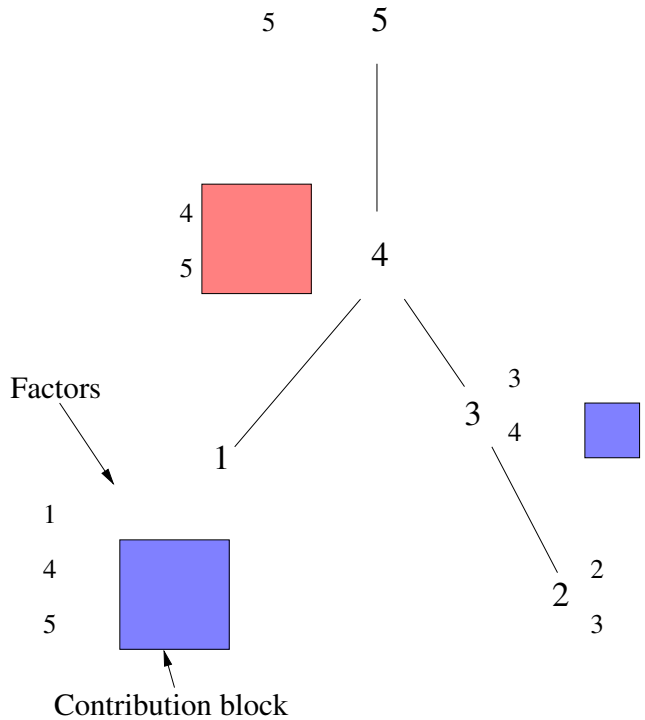

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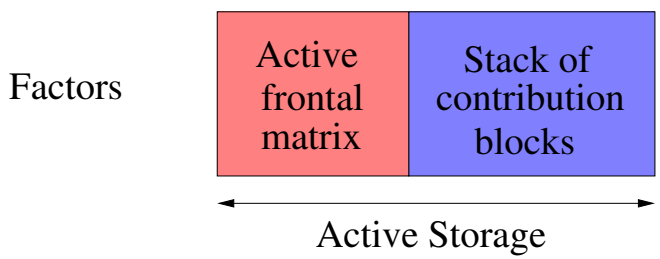

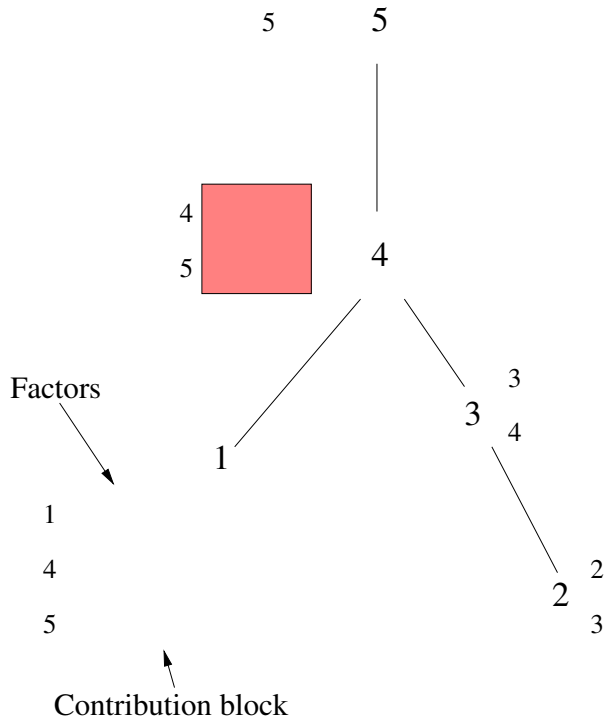

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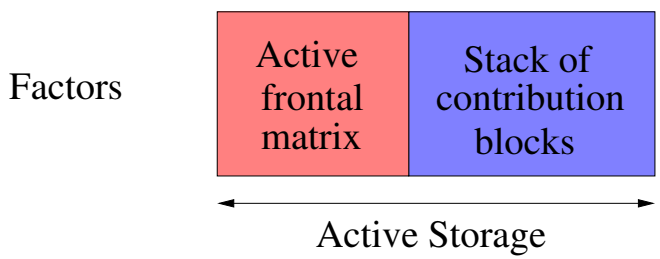

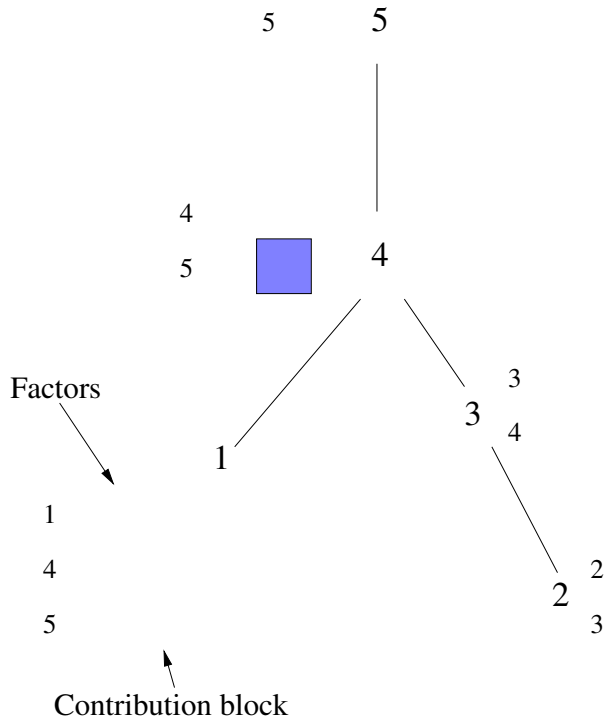

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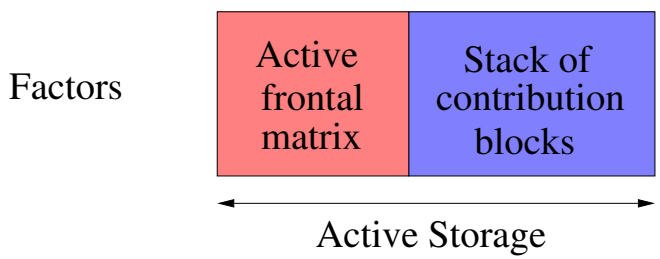
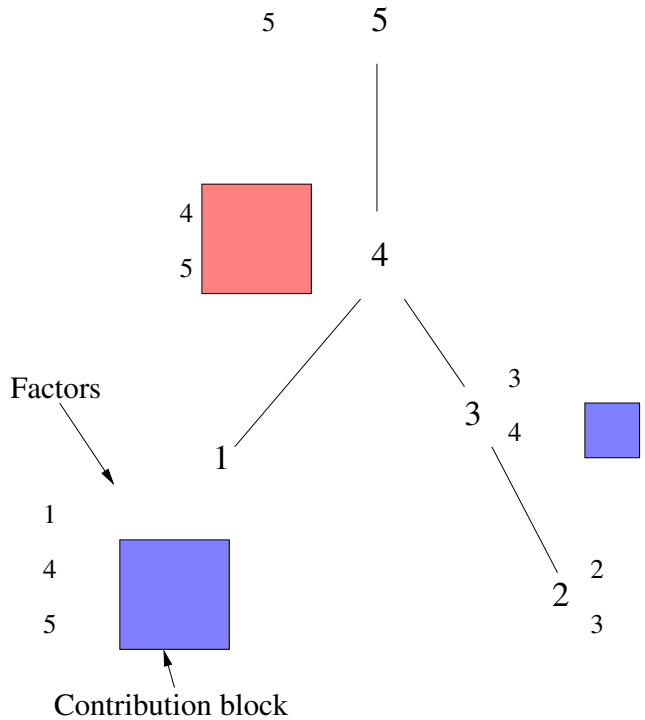
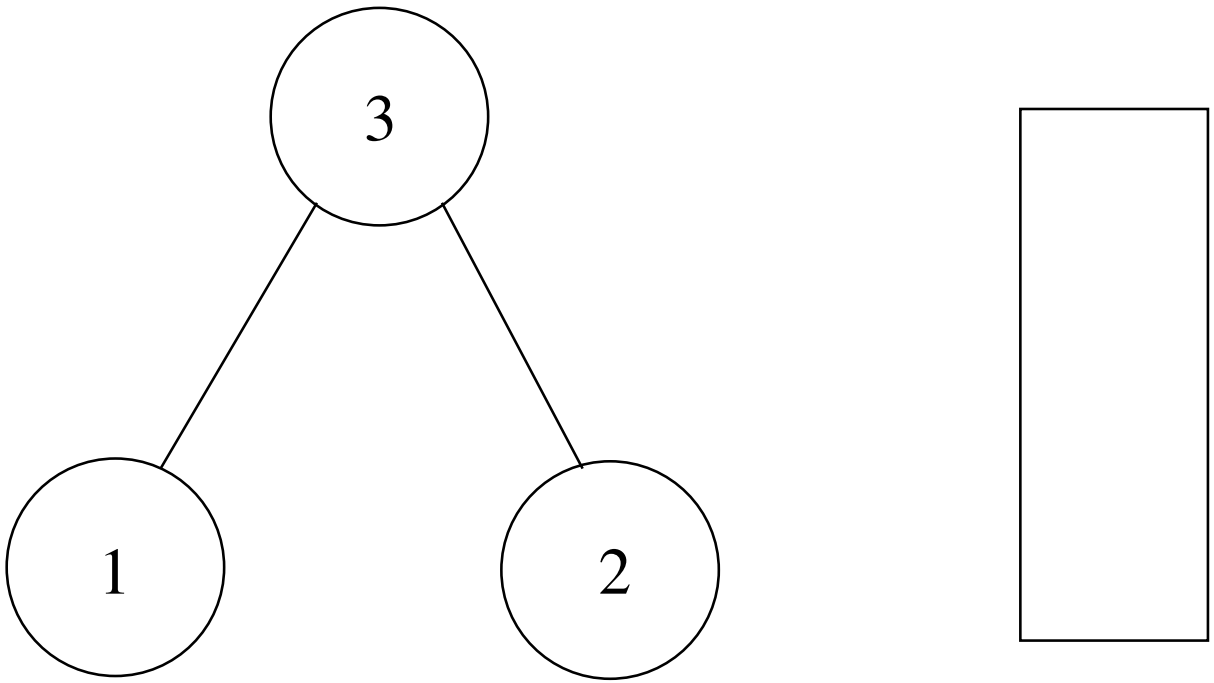




Elimination tree

Memory Behaviour (serial postorder traversal)



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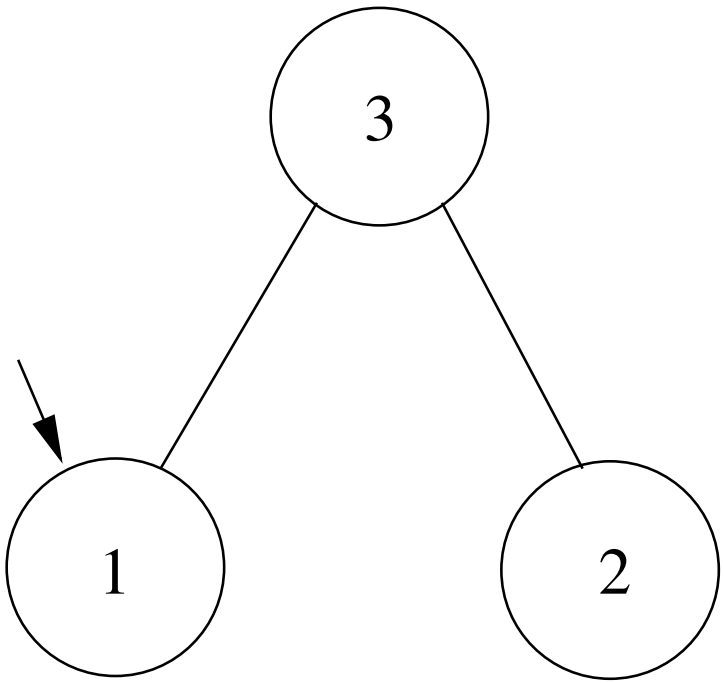

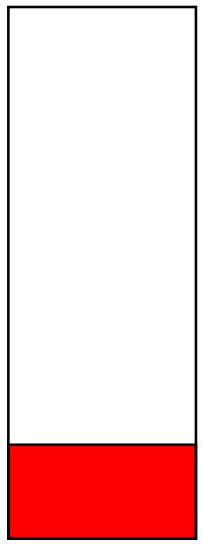

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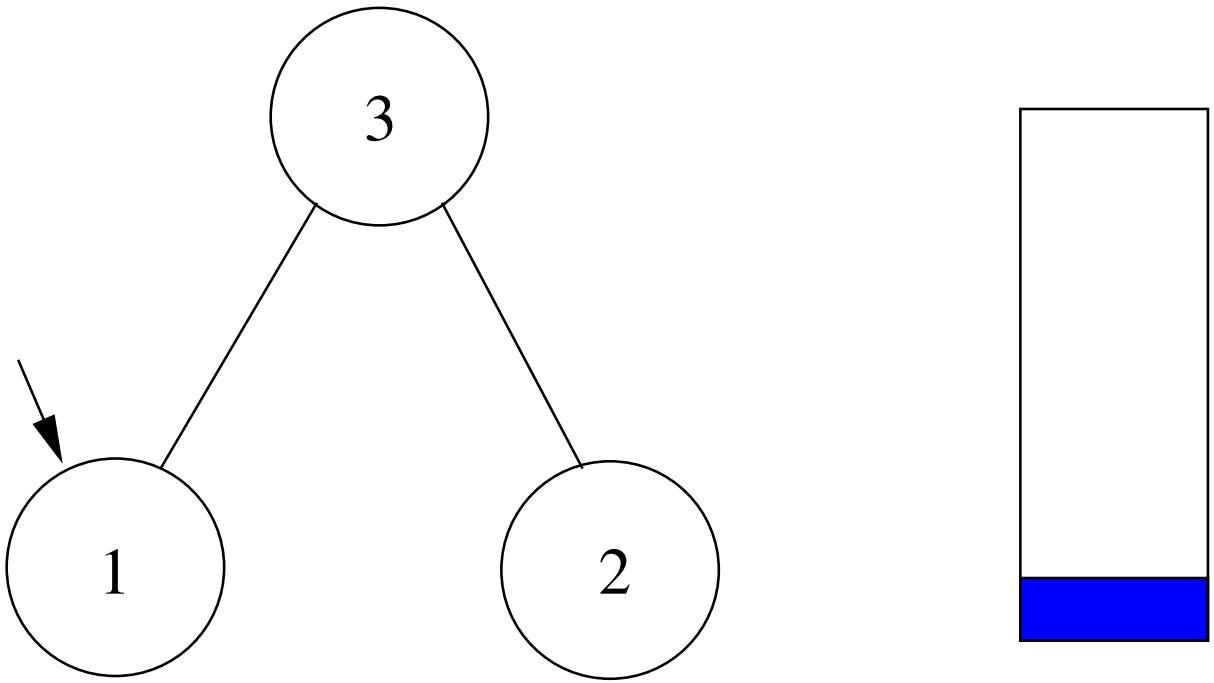

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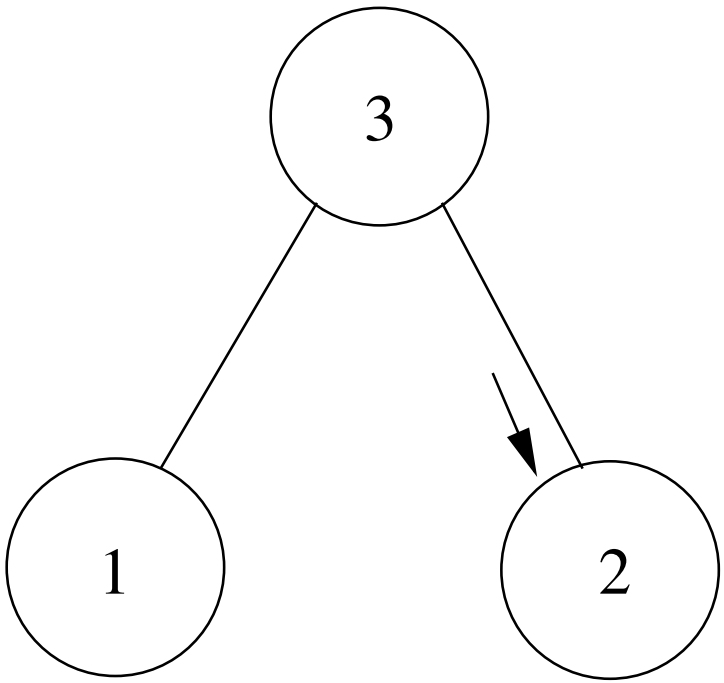

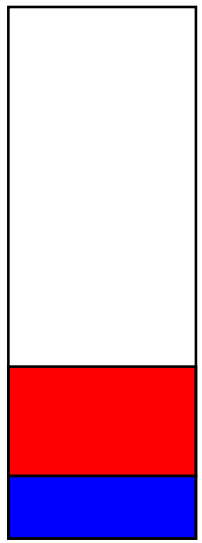

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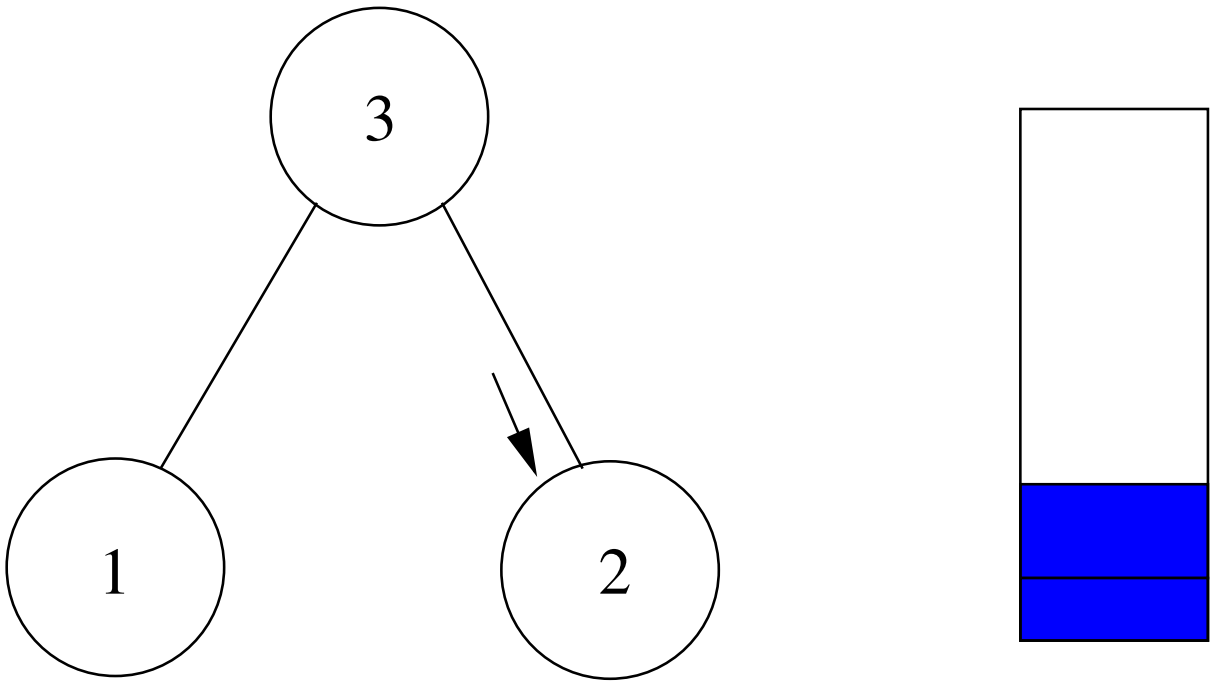

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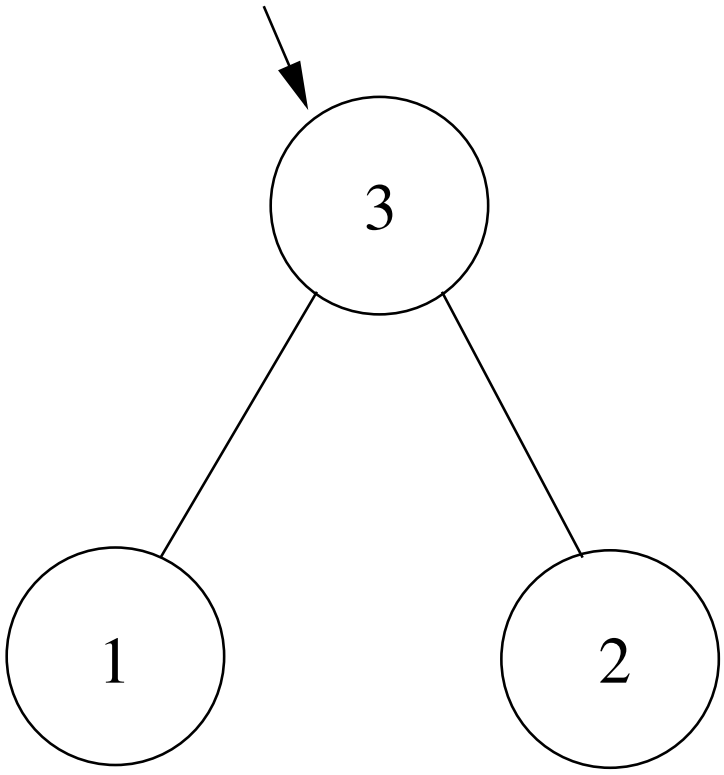

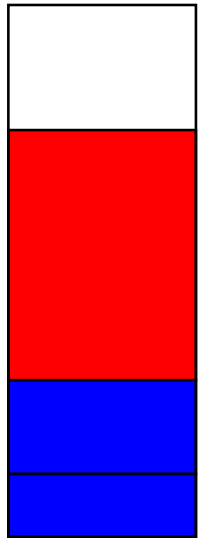

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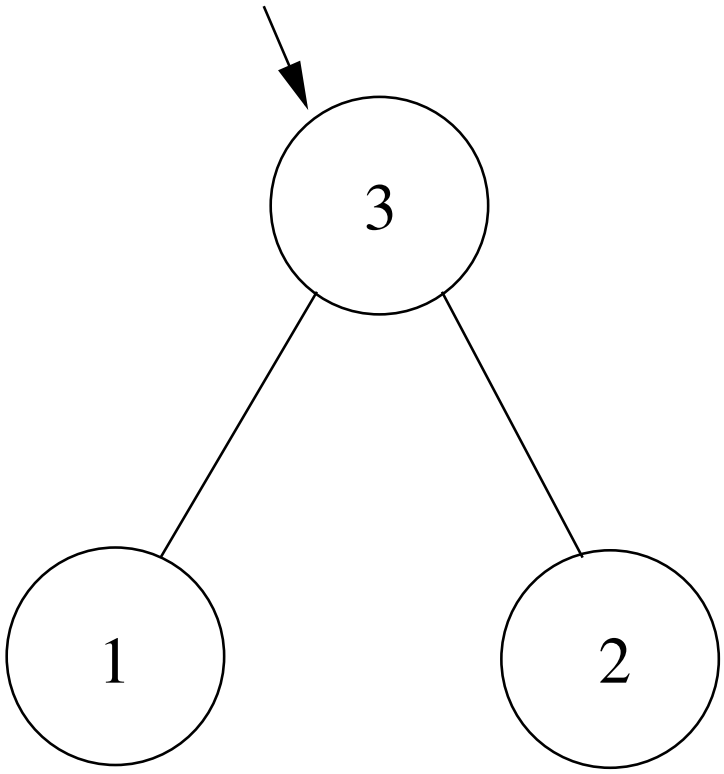

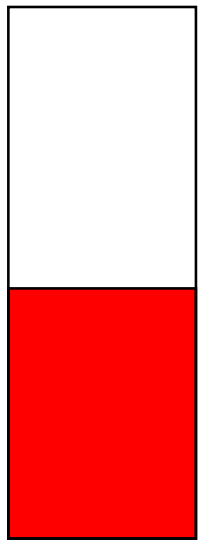

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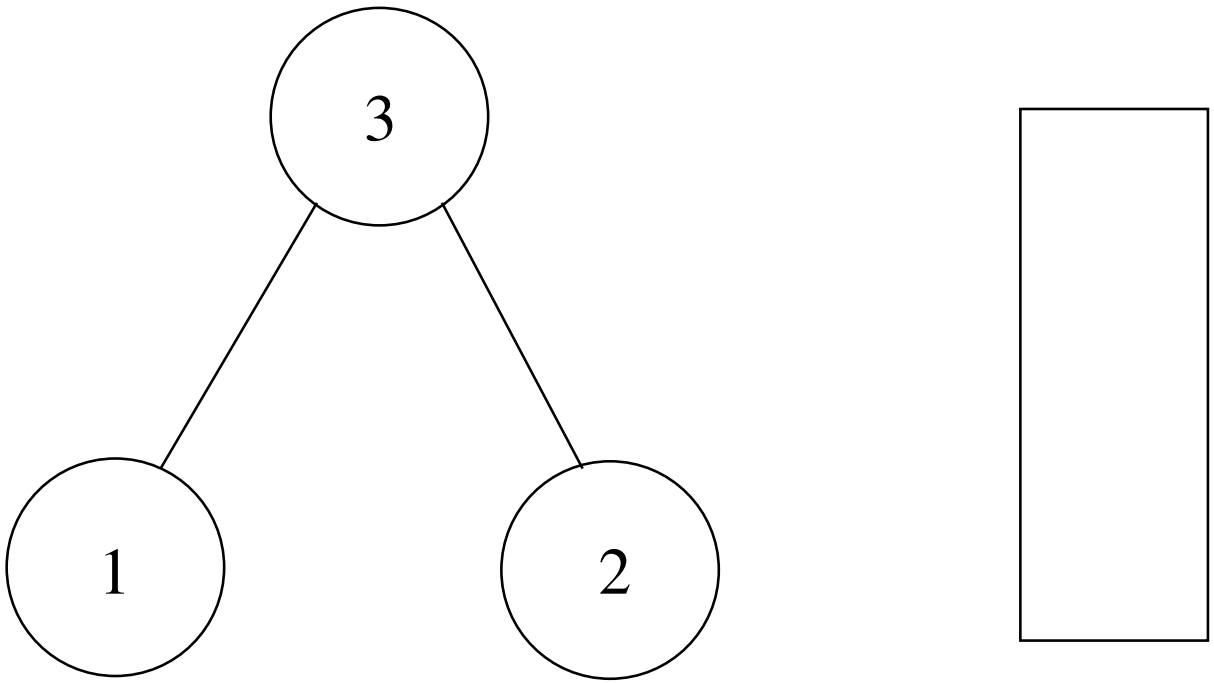
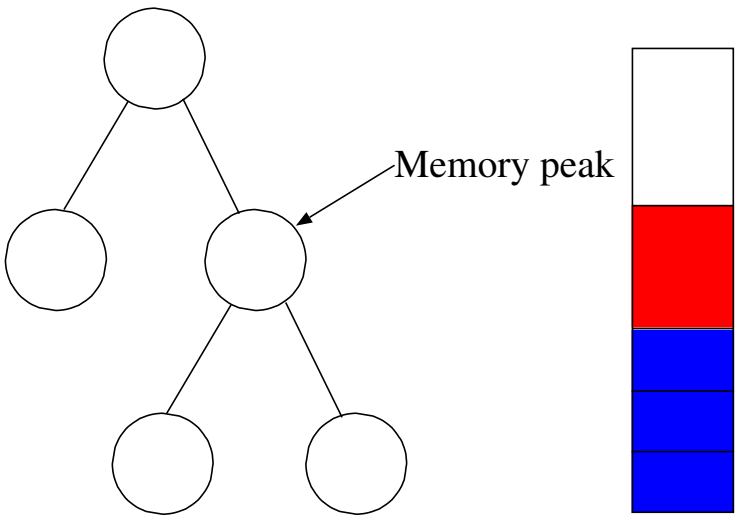
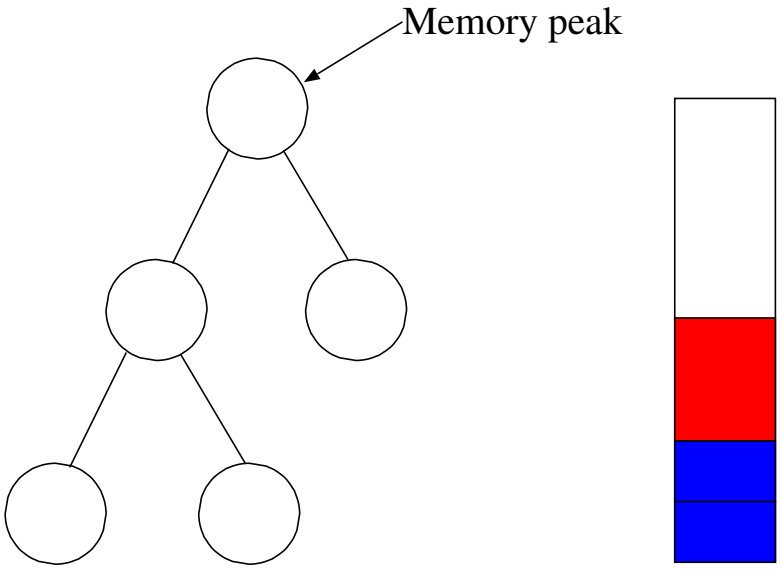


Sequential case results



Worst case.



Best case.

→ Algorithms to find the optimal tree traversal have been proposed

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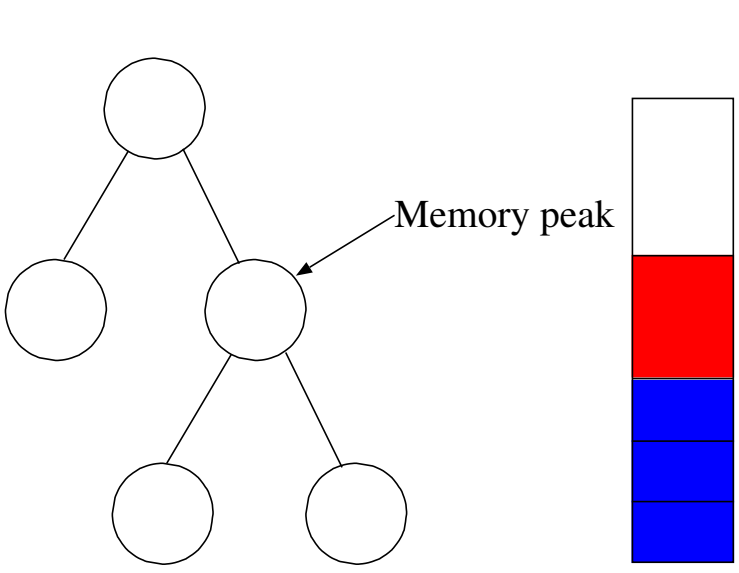

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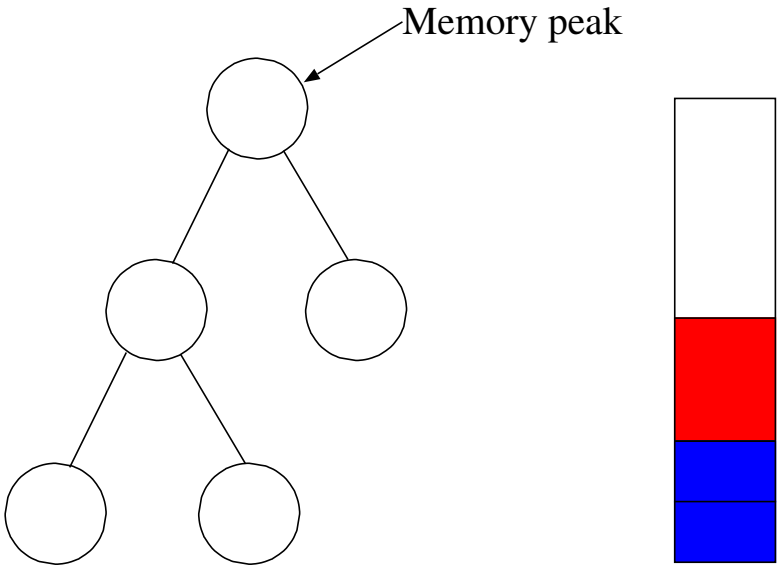

Best case.

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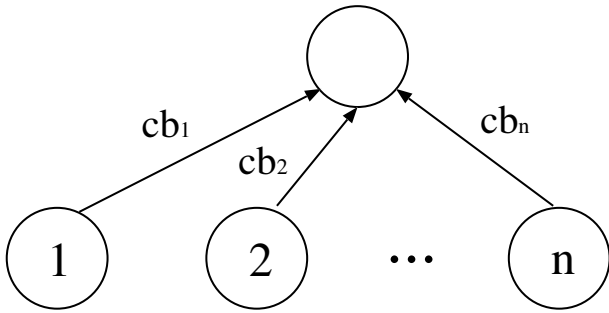
Sequential case: Memory Behavior (2/2)

Consider a parent node in the tree:

- n is the number of children.
- j denotes the j^{th} child of the node.
- cb_j is the size of the contribution block of child j.
- m is the memory size of the frontal matrix of the parent.
- A (resp. A_j) is the amount of active memory needed to process the parent (resp. child j).



The assembly step requires a storage:

$$m + \sum_{j=1}^{n} cb_j$$

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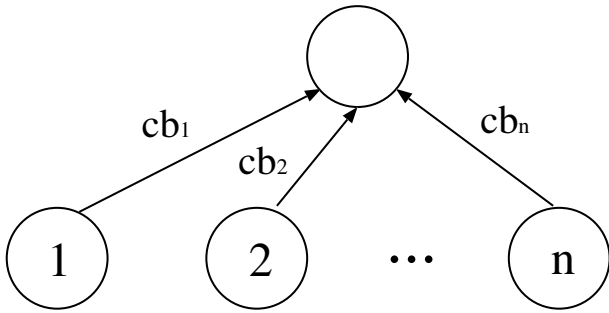

The storage required to process child j is:

$$A_j + \sum_{k=1}^{j-1} cb_k$$

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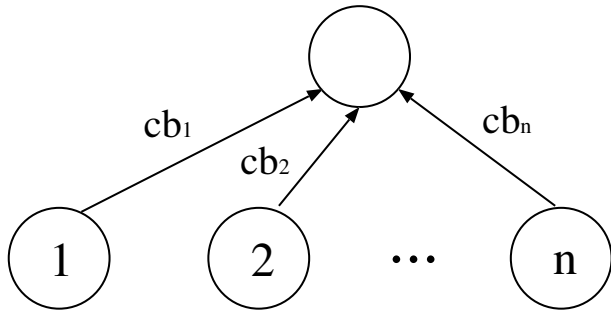


A is thus defined by:

$$A = \max(\max_{j=1,n}(A_j + \sum_{k=1}^{j-1} cb_k), m + \sum_{j=1}^{n} cb_j)$$

Outline

Liu's Algorithm

Liu's Theorem (Tree pebbling theorem)

The minimum of $\max_j(x_j + \sum_{i=1}^{j-1} y_j)$ *is obtained when the sequence* (x_i, y_i) *is sorted in decreasing order of* $x_i - y_i$,

Consequence:

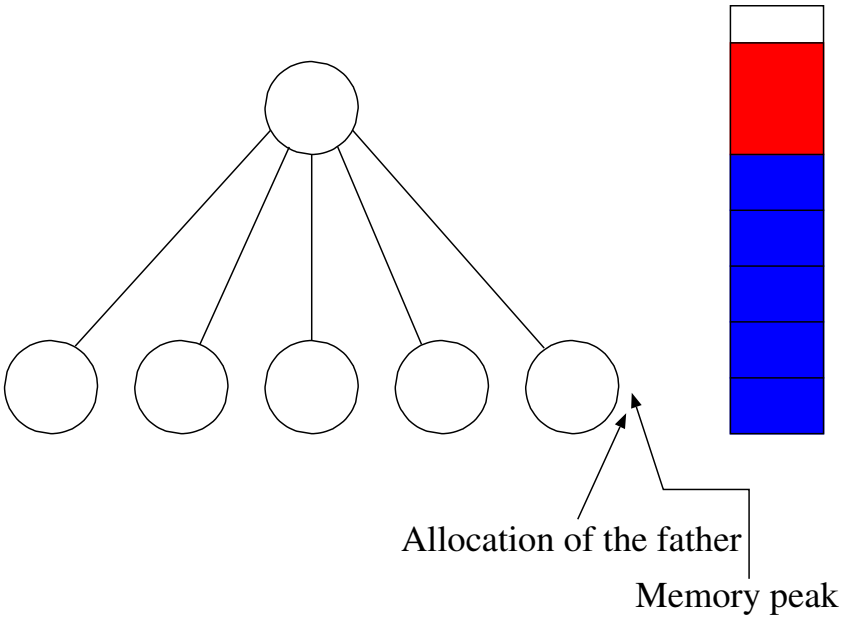
An optimal child sequence is obtained by rearranging the children nodes in decreasing order of $A_i - cb_i$.

Algorithm:

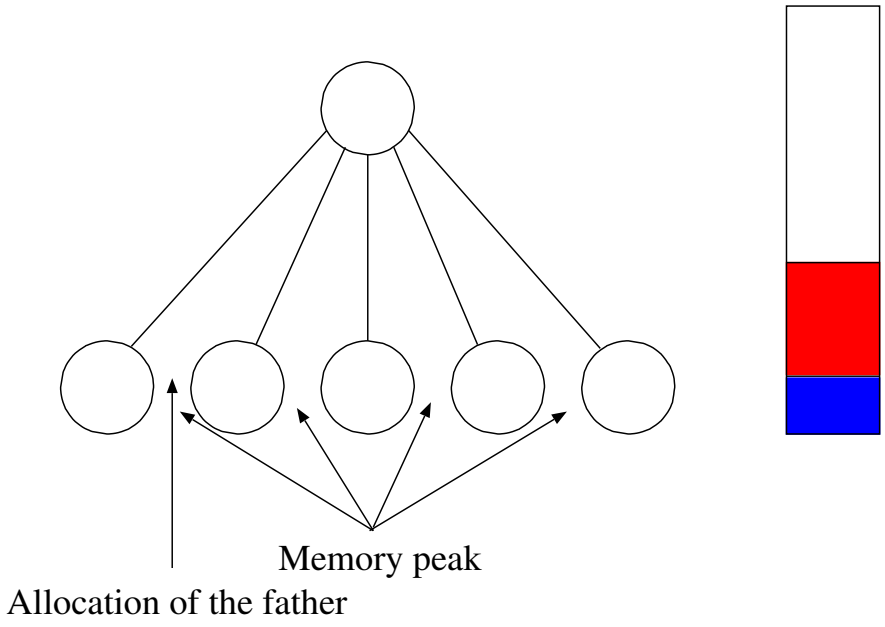
- Bottom-up greedy process.
- Apply Liu's theorem at each level of the tree.

Outline

Limitation of the Classical scheme



Classical approach.



Flexible scheme.

→ Decoupling the allocation and the computations can improve the memory behavior

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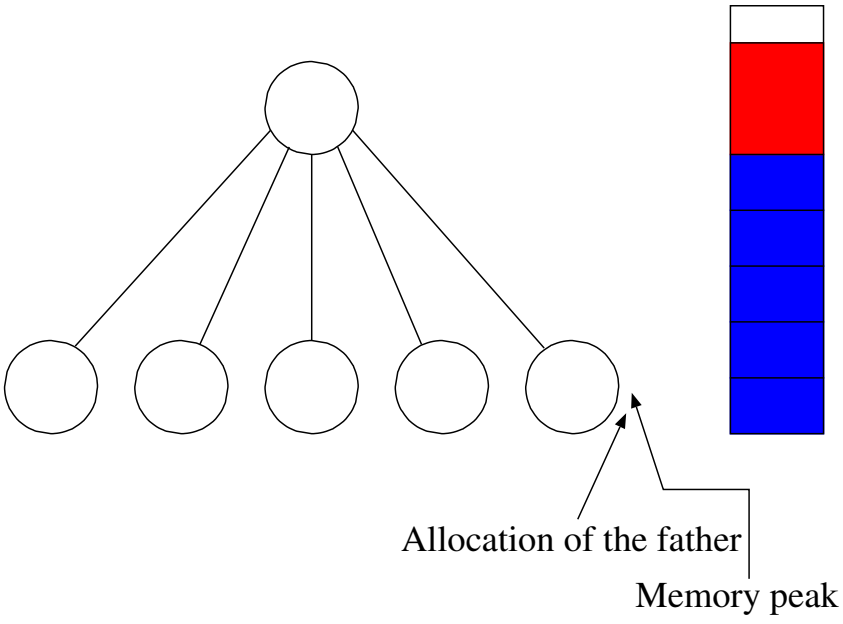

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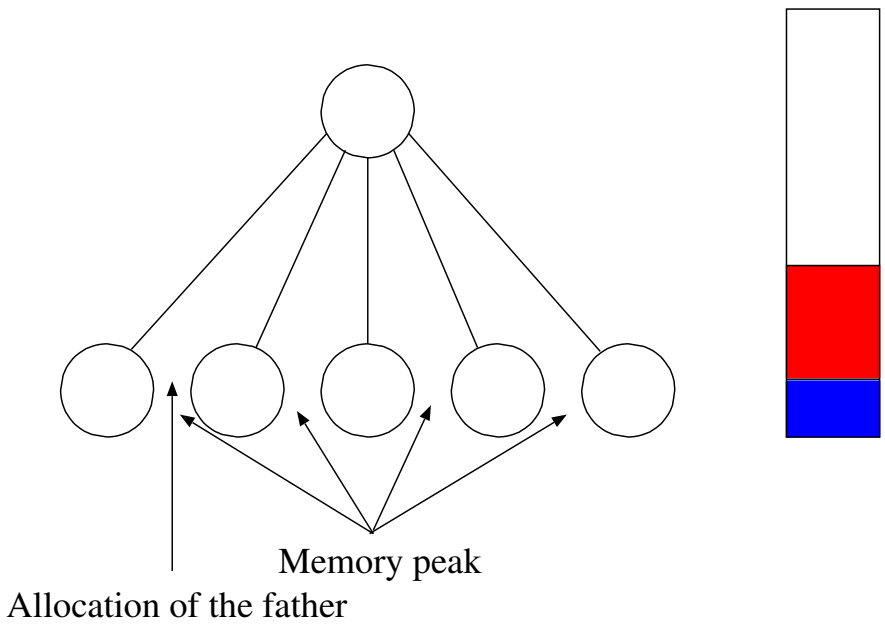

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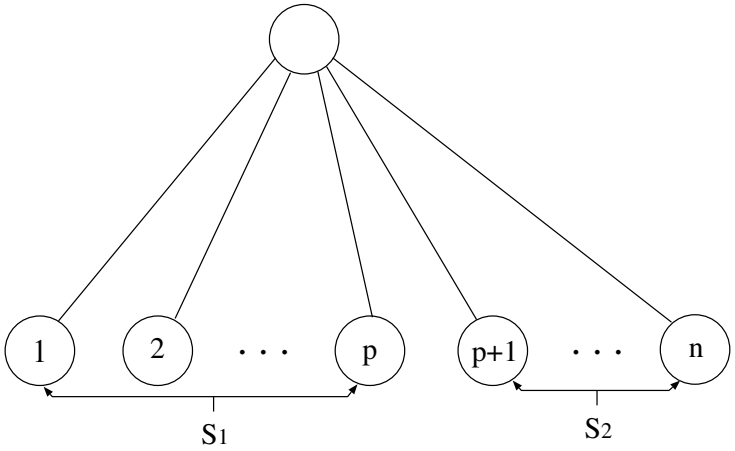
Flexible multifrontal scheme

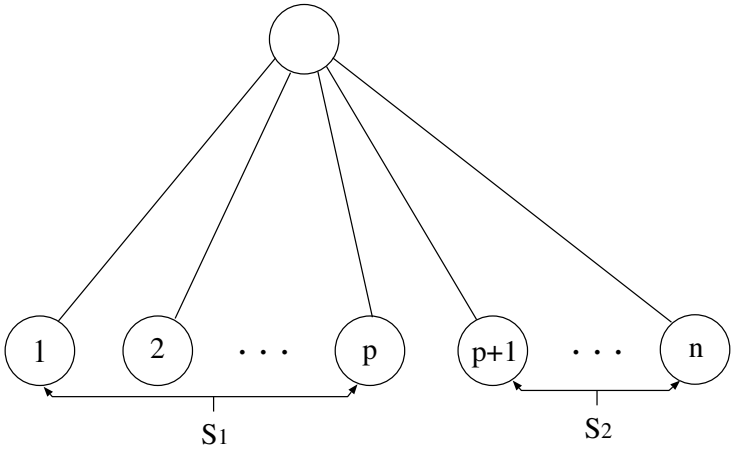


- p is the position of the allocation of the parent.
- $\mathcal{S}_1$ is the set of children treated before the allocation of the parent.
- $\mathcal{S}_2$ is the set of children treated after the allocation of the parent.

- The memory behavior inside $\mathcal{S}_1$ is similar to the case of the classical multifrontal scheme.
- Inside $\mathcal{S}_2$, the order of the children has no impact on the memory behavior.

$$A^{flex} = \max\left(\max_{j=1,p}(A_j^{flex} + \sum_{k=1}^{j-1} cb_k), m + \sum_{k=1}^{p} cb_k, m + \max_{j=p+1,n} A_j^{flex}\right)$$

Flexible multifrontal scheme



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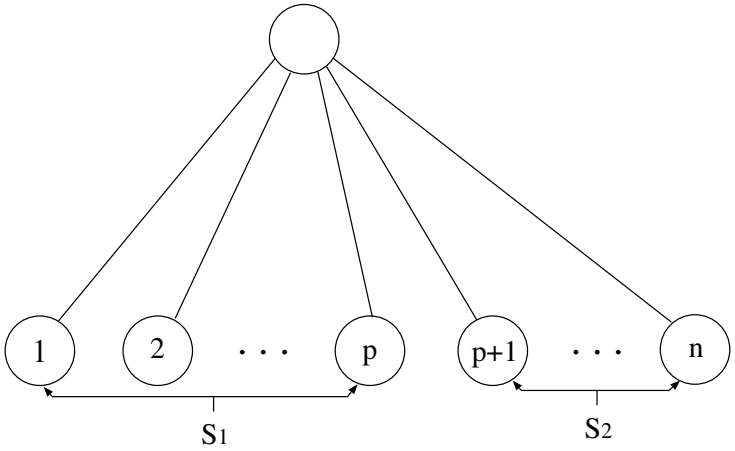

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A new memory minimization algorithm

Theorem

An optimal sequence can be obtained by :

- *Sorting the children in decreasing order of* A_j^{flex}.
- *Trying all the possible positions for the allocation of the parent and sorting the children belonging to* $\mathcal{S}_1$ *according to Liu's Theorem.*
- *Selecting the configuration that gives the smallest peak.*

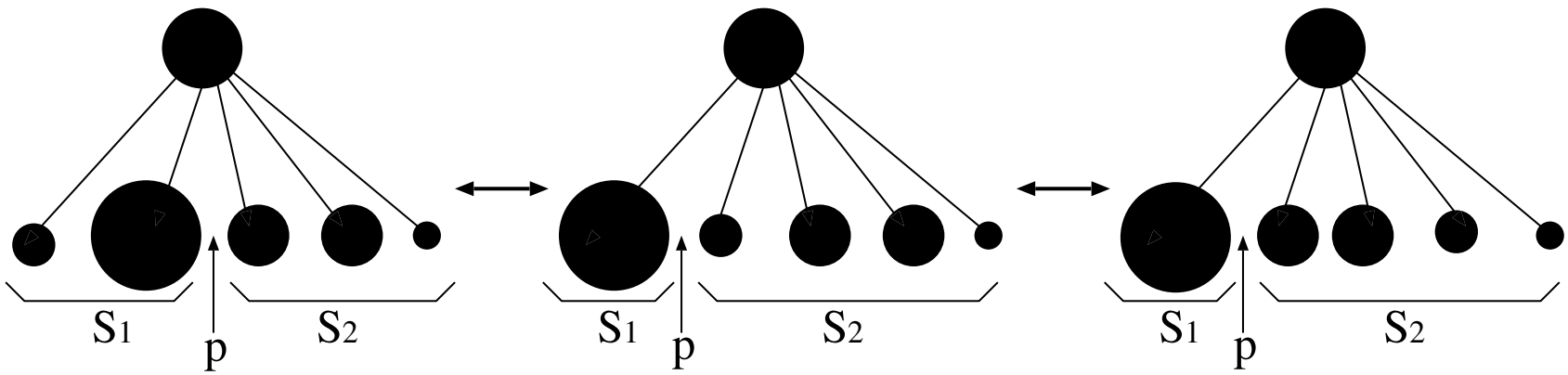
Algorithm:

Bottom-up greedy process where the theorem is applied at each level of the tree.

Proof

$$A^{flex} = \max\left(\max_{j=1,p}(A_j^{flex} + \sum_{k=1}^{j-1} cb_k), m + \sum_{k=1}^{p} cb_k, m + \max_{j=p+1,n} A_j^{flex}\right)$$

- Inside $\mathcal{S}_2$, the order of the children has no impact on the memory behavior.
- If $\exists j \in \mathcal{S}_1 \,/\, A_j^{flex} \leq \max_{i \in \mathcal{S}_2}(A_i^{flex}) \rightarrow j$ can be moved from $\mathcal{S}_1$ to $\mathcal{S}_2$ without increasing the peak.



Optimal configuration

Active memory minimization Algorithm

Algorithm:

Set $\mathcal{S}_1 = \{1, \ldots, n\}$, $\mathcal{S}_2 = \emptyset$ and $p = n$;
Find the schedule providing an optimal A^{flex} value for partition $(\mathcal{S}_1, \mathcal{S}_2)$;
repeat
  Find j such that $A_j^{flex} = \min_{k \in \mathcal{S}_1} A_k^{flex}$;
  Set $\mathcal{S}_1 = \mathcal{S}_1 \setminus \{j\}$, $\mathcal{S}_2 = \mathcal{S}_2 \cup \{j\}$, and $p = p - 1$;
  Find the schedule providing an optimal A'^{flex} value for partition $(\mathcal{S}_1, \mathcal{S}_2)$;
  if $A'^{flex} \leq A^{flex}$ **then**
    Keep the value of p, and the schedule of children in $\mathcal{S}_1$ and $\mathcal{S}_2$ corresponding to A'^{flex};
    Set $A^{flex} = A'^{flex}$;
  end if
until $p == 1$ or $A'^{flex} > A^{flex}$

Outline

Experimental environment

MUMPS: Multifrontal Parallel Solver for both LU and LDL^T.
Reordering techniques: *AMD*, *AMF*, *METIS*, *PORD*.
Test platform: *IBM* platform at *IDRIS*.
Test problems: Large range of matrices extracted from various collections (Rutherford-Boeing, University of Florida or PARASOL,...).
Schedules tested :

- Classical multifrontal scheme (parent allocated after all its children).
- Anticipated parent allocation scheme (parent allocated after its first child).
- Flexible parent allocation scheme (parent allocated at an arbitrary position).

Simulation of memory variations for all the schedules during the analysis step.

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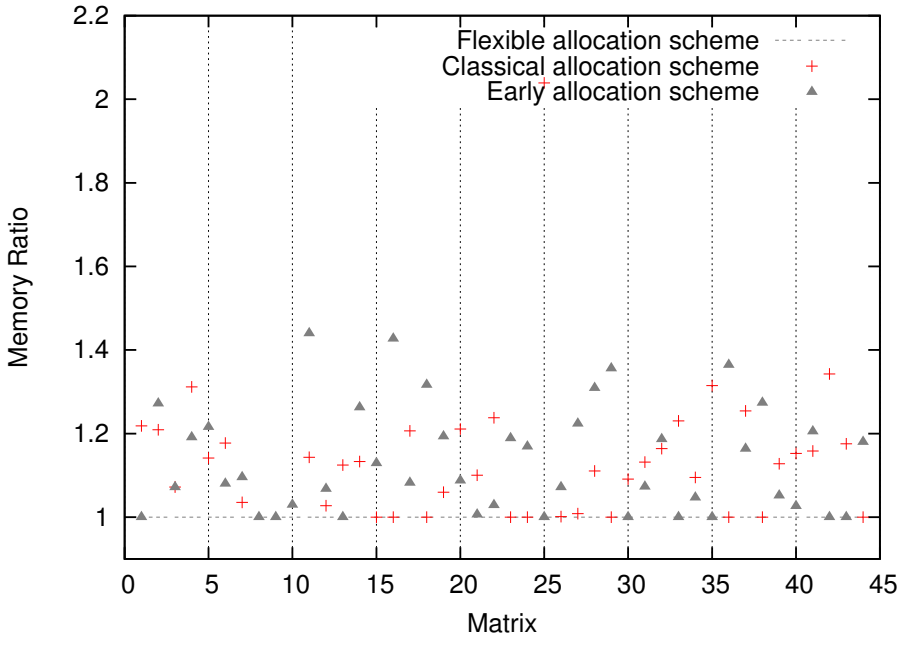
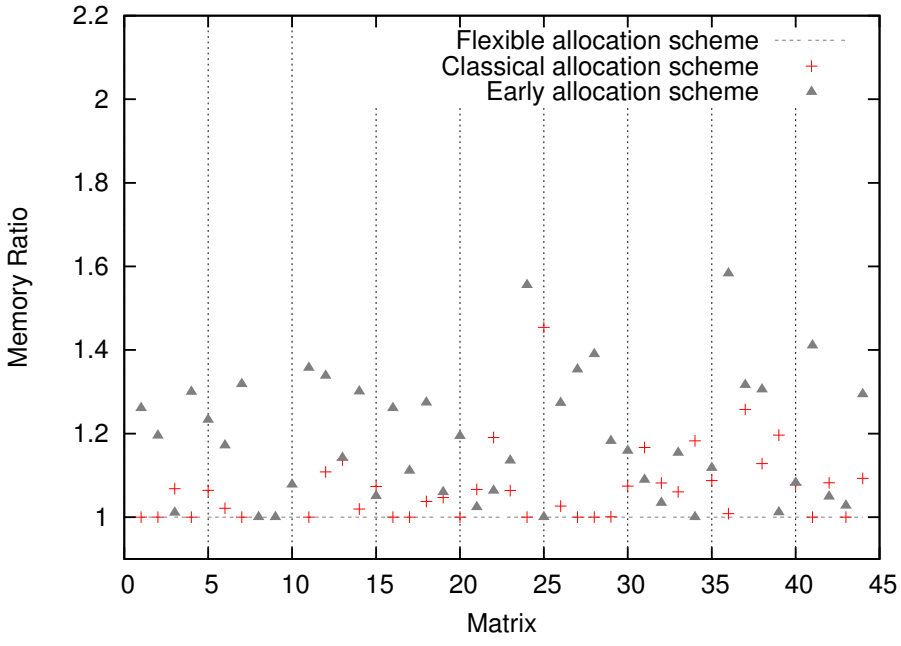
Experimental results: Active memory gains



AMD.



METIS.

Large gains against the *classical allocation scheme* for matrices 8, 9 and 10.

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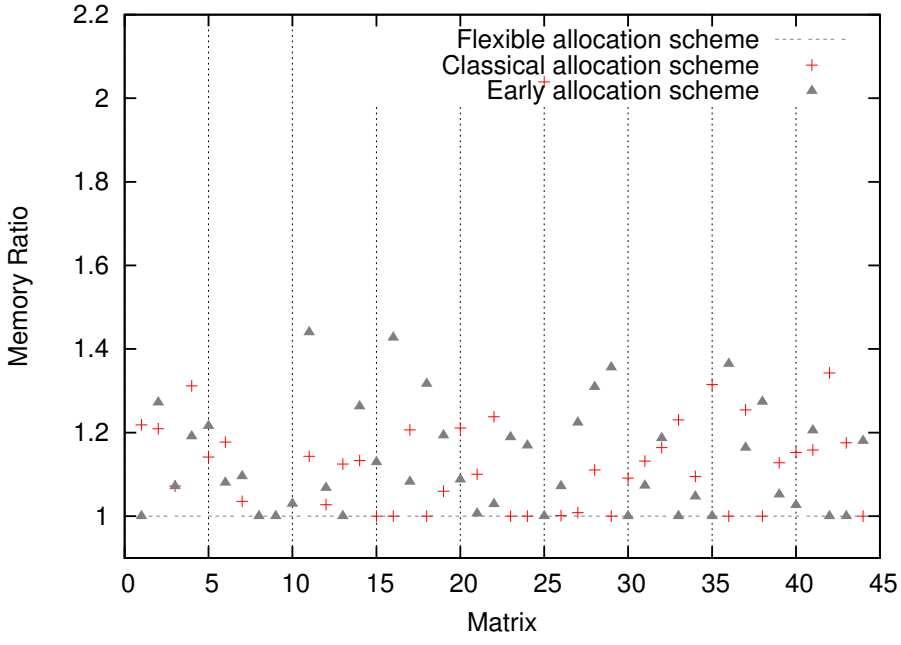

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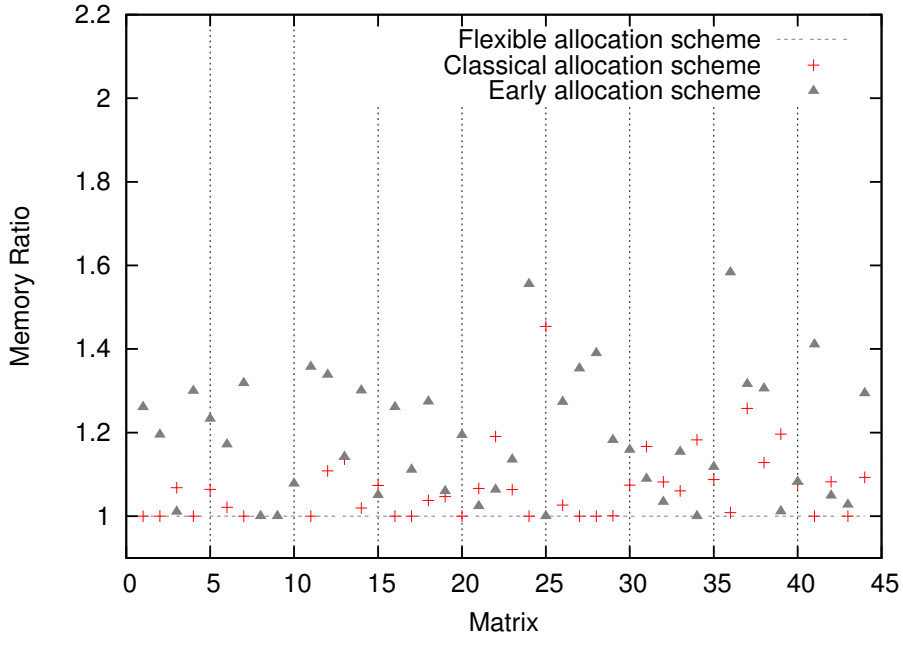

METIS.

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Outline

Total memory minimization (1/3)

Memory space T^{flex} needed for the processing of a node in the tree is given by:

$$\mathcal{P}_1 = \max\Big(\max_{j=1,p}(T_j^{flex} + \sum_{k=1}^{j-1}(cb_k + F_k)),$$

$$m + \sum_{k=1}^{p}(cb_k + F_k)\Big)$$

$$\mathcal{P}_2 = \max\Big(m + \sum_{k=1}^{p} F_k + \max_{j=p+1,n}(T_j^{flex} + \sum_{k=p+1}^{j-1} F_k)\Big)$$

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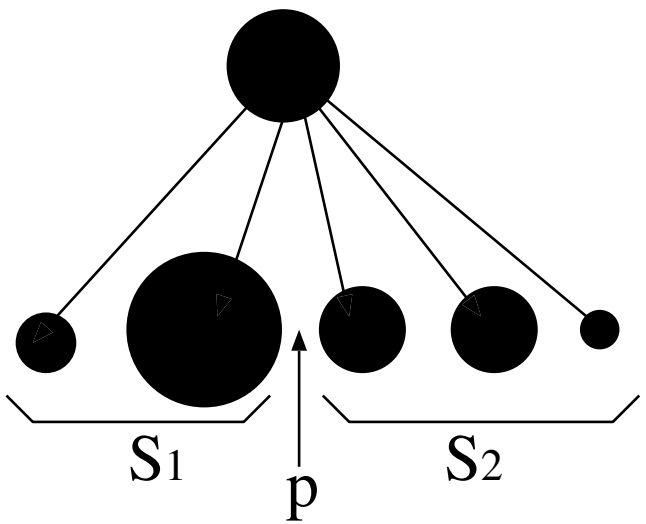
Total memory minimization (2/3)

	$\mathcal{S}_1$	$\mathcal{S}_2$
Children sequence	$T_i^{flex} - (cb_i + F_i)$	$T_i^{flex} - F_i$

Total memory minimizing sequences inside $\mathcal{S}_1$ and $\mathcal{S}_2$.

Property:



let $j_0 \in \mathcal{S}_2$ be the child for which the peak is reached inside $\mathcal{S}_2$. $\rightarrow$ The total memory peak cannot decrease if j_0 remains in $\mathcal{S}_2$ for all configurations where $\mathcal{S}_1 \subset \mathcal{S}'_1$.

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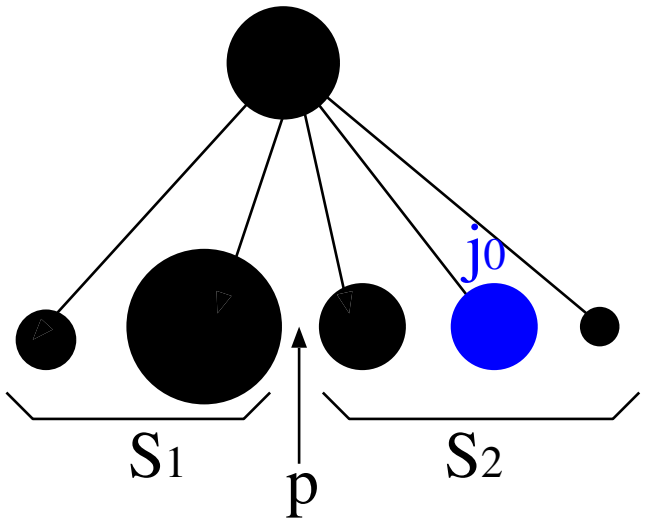

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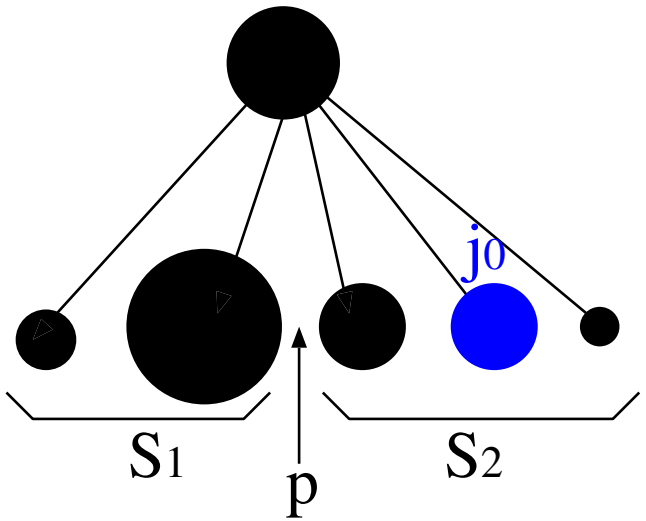

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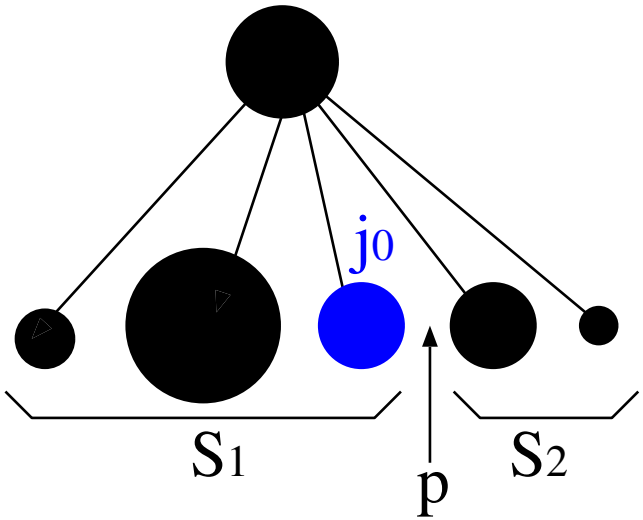

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Total memory minimization (3/3)

Algorithm:

Set $\mathcal{S}_1 = \emptyset$, $\mathcal{S}_2 = \{1, \ldots, n\}$ and $p = 0$;
Sort $\mathcal{S}_2$ according in decreasing order of $T_j^{flex} - F_j$;
Compute $T^{flex} = \mathcal{P}_2$;
repeat
  Find j_0 such that the peak in $\mathcal{P}_2$ is obtained for j_0;
  Set $\mathcal{S}_1 = \mathcal{S}_1 \cup \{j_0\}$, $\mathcal{S}_2 = \mathcal{S}_2 \setminus \{j_0\}$, and $p = p + 1$;
  (Remark: j_0 is inserted at the position in $\mathcal{S}_1$ so that the order inside this set is decreasing in terms of $T_j^{flex} - (cb_j + F_j)$.)
  Compute $\mathcal{P}_1$, $\mathcal{P}_2$, and $T'^{flex} = \max(\mathcal{P}_1, \mathcal{P}_2)$;
  if $T'^{flex} \leq T^{flex}$ **then**
    Keep the values of p, $\mathcal{S}_1$ and $\mathcal{S}_2$ and set $T^{flex} = T'^{flex}$;
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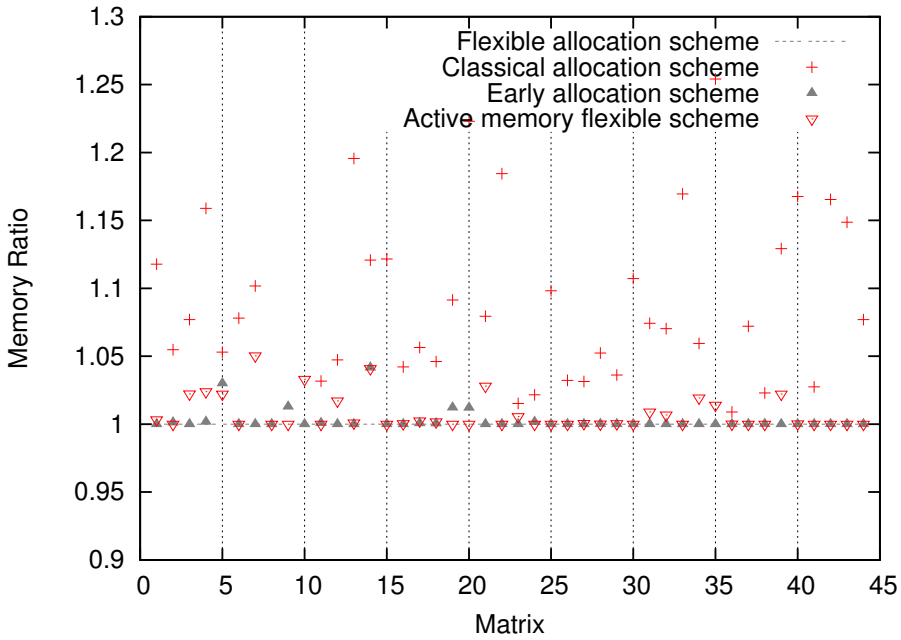
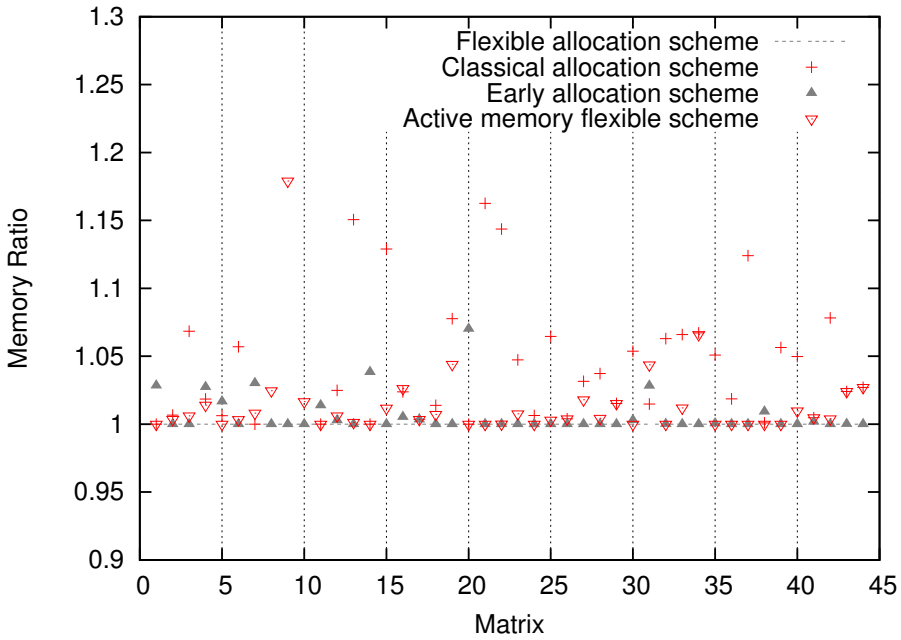
Experimental results: Total memory gains



AMD.

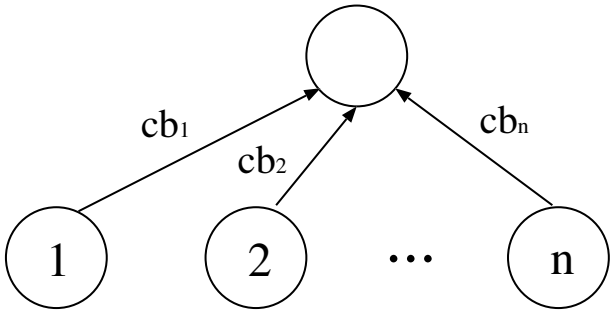


METIS.

Outline

Outline

Notations et assumptions



- M_0: Core memory available
- m: Size of the frontal matrix of the parent ($m < M_0$)
- n: Number of children
- i: i^{th} child
- cb_i: Size of the contribution block of child i
- M_i: Memory required to process the subtree rooted at child i

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- Factors are written to disk as soon as computed
- Each frontal matrix fits in core memory (*i.e.* $m < M_0$)
- Oldest CBs written first

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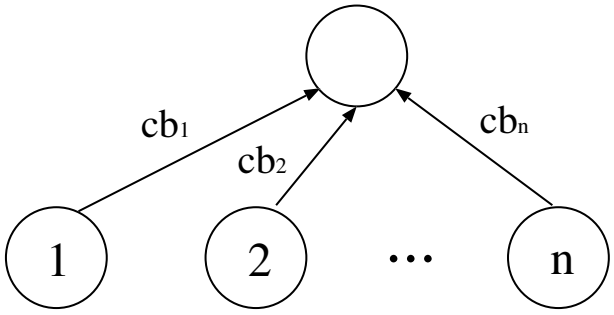

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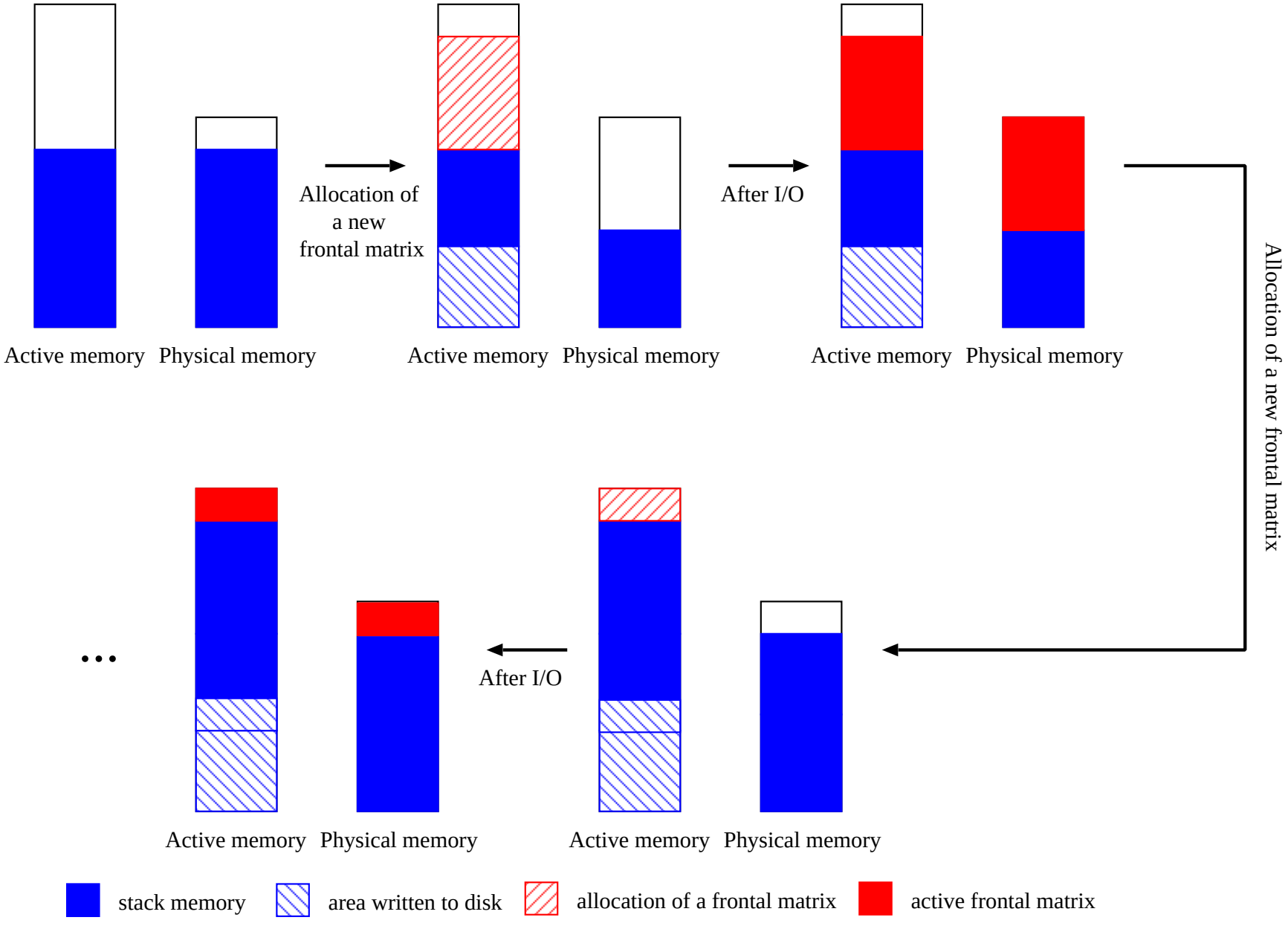
I/O volume (1/3)


Allocation of
a new
frontal matrix
After I/O
Allocation of a new frontal matrix
Active memory
Physical memory
Active memory
Physical memory
Active memory
Physical memory
...
After I/O
Active memory
Physical memory
Active memory
Physical memory
stack memory
area written to disk
allocation of a frontal matrix
active frontal matrix

I/O volume (2/3)

Let be a parent and its children

Case 1: $\forall i \in 1;...;n : M_i < M_0$

I/O produced at assembly step:

$$\max(0, m + \sum_{j=1}^{n} cb_j - M_0)$$

I/O produced when processing the subtree rooted at child j:

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$V^{I/O}$ is thus:

$$V^{I/O} = \max\left(\max_{j=1,n}\left(\max(M_j + \sum_{k=1}^{j-1} cb_k), m + \sum_{j=1}^{n} cb_j\right) - M_0, 0\right)$$

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I/O volume (3/3)

Case 2: General case ($\exists i \in 1;...;n : M_i > M_0$)

- Same expression for the active memory
- New expression for the *I/O* volume:
  - If $M_i > M_0$ then:
    1. $V_i^{I/O}$ independent of position of child i
    2. When processing child i, CBs of previously processed children are written to disk

$$V^{I/O} = \max\left(\max_{j=1,n}(\min(M_j, M_0) + \sum_{k=1}^{j-1} cb_k), m + \sum_{j=1}^{n} cb_j\right) - M_0 + \sum_{i=1}^{n} V_i^{I/O}$$

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$\Longrightarrow$ Total *I/O* volume computed with a greedy depth-first traversal on the whole tree

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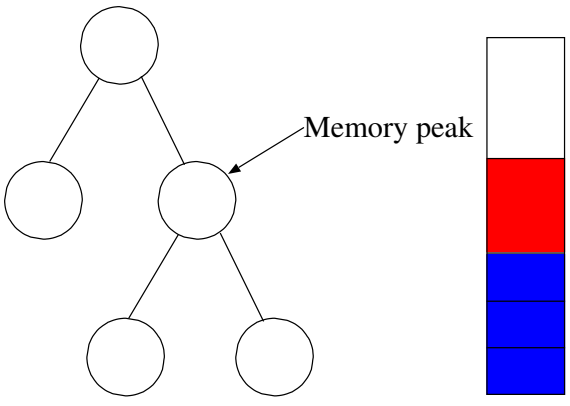
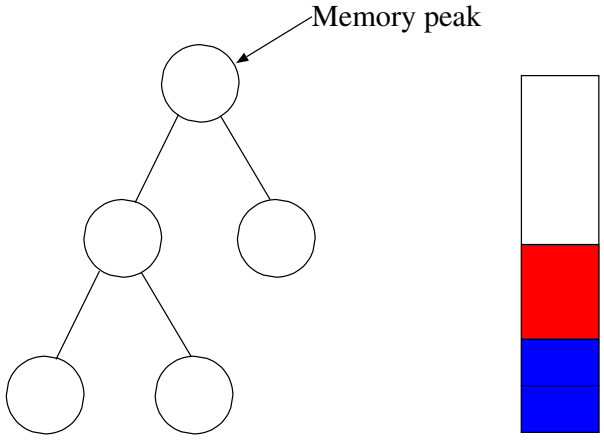
Outline

Problem

- Assumption: factors written to disk as soon as computed
- Active memory peak: tree traversal-dependent



Worst case



Best case

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- Problem: How to minimize the *I/O* volume when the active memory does not hold in a given amount of physical memory M_0 ?

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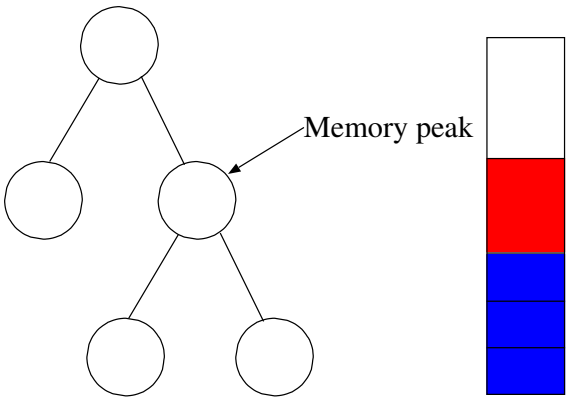

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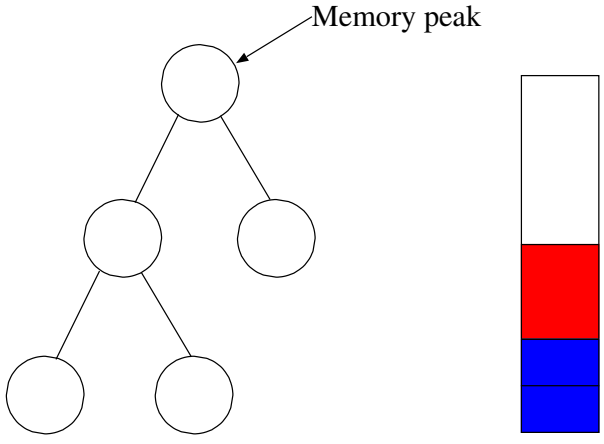

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Minimizing I/O volume

How to process the children to minimize $V^{I/O}$?

- Minimizing $V^{I/O}$ corresponds to minimize:

$$\max_{j=1,n}\left(\min(M_j, M_0) + \sum_{k=1}^{j-1} cb_k\right)$$

Theorem (Tree pebbling theorem)

The minimum for $\max_j(x_j + \sum_{i=1}^{j-1} y_j)$ is obtained when the sequence (x_j, y_j) is sorted in the increasing order of $x_j - y_j$.

Consequence: An optimal sequence is got by ordering the children nodes in the increasing order of $\min(M_j, M_0) - cb_j$.

- Algorithm:
  - Greedy depth-first traversal process
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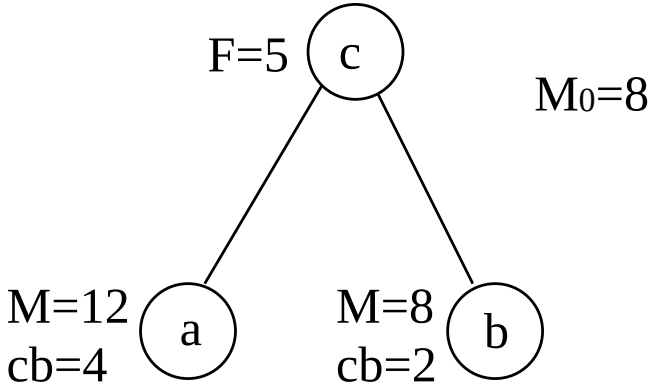
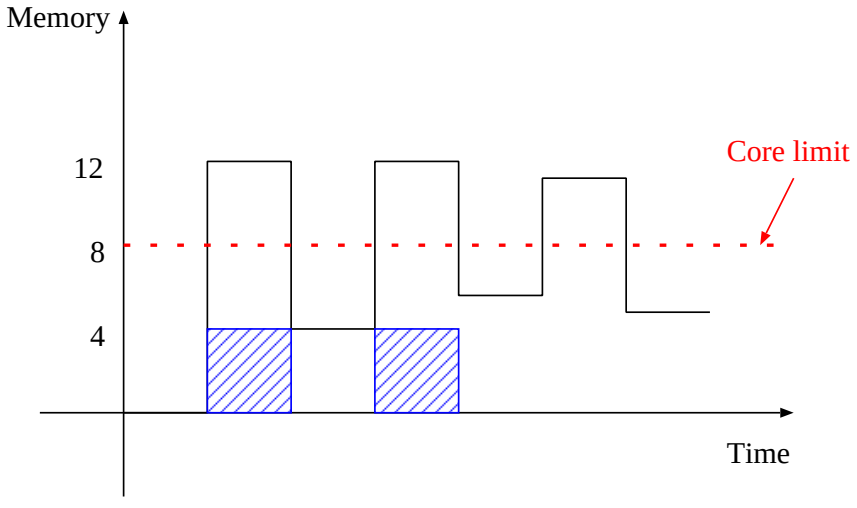
Toy example



Liu's Algorithm

sequence $\rightarrow$ a-b-c

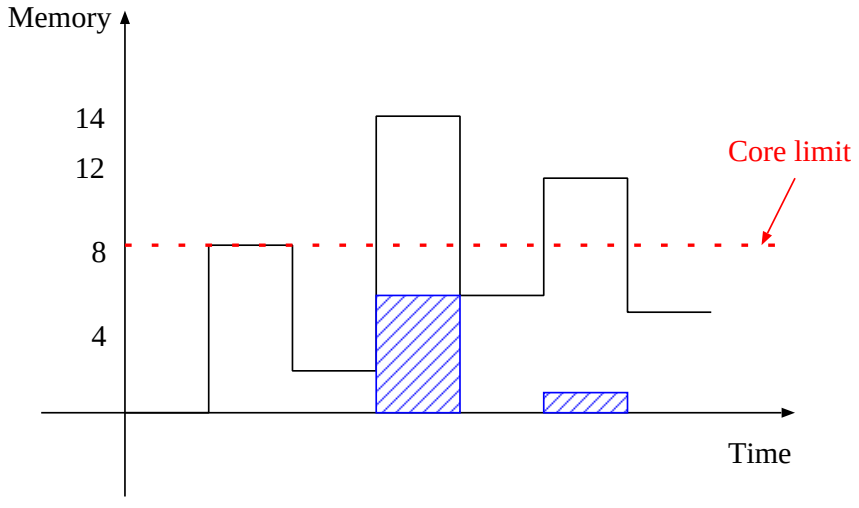
$A_{fath} = 12,\ V^{I/O} = 8$



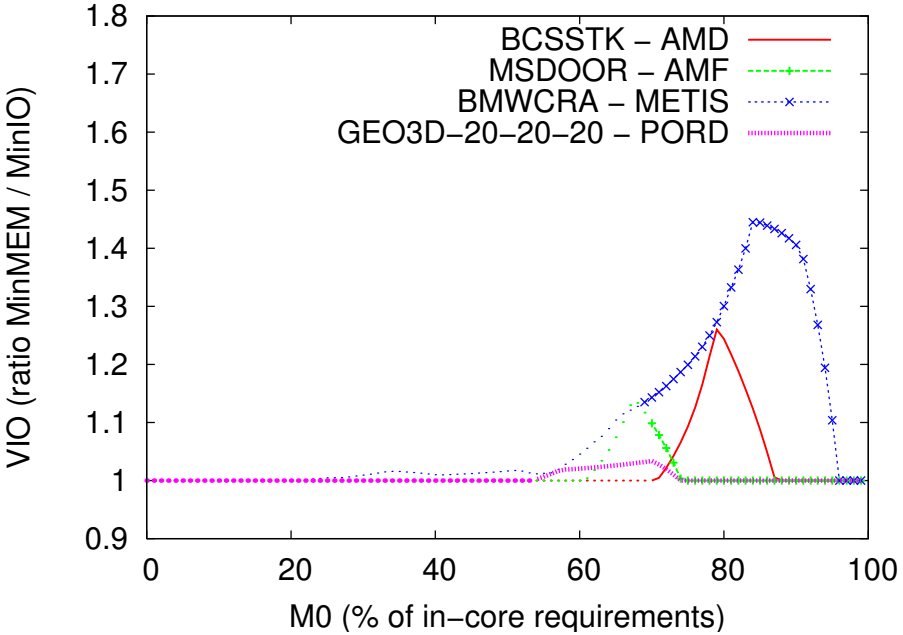
I/O minimization Algorithm

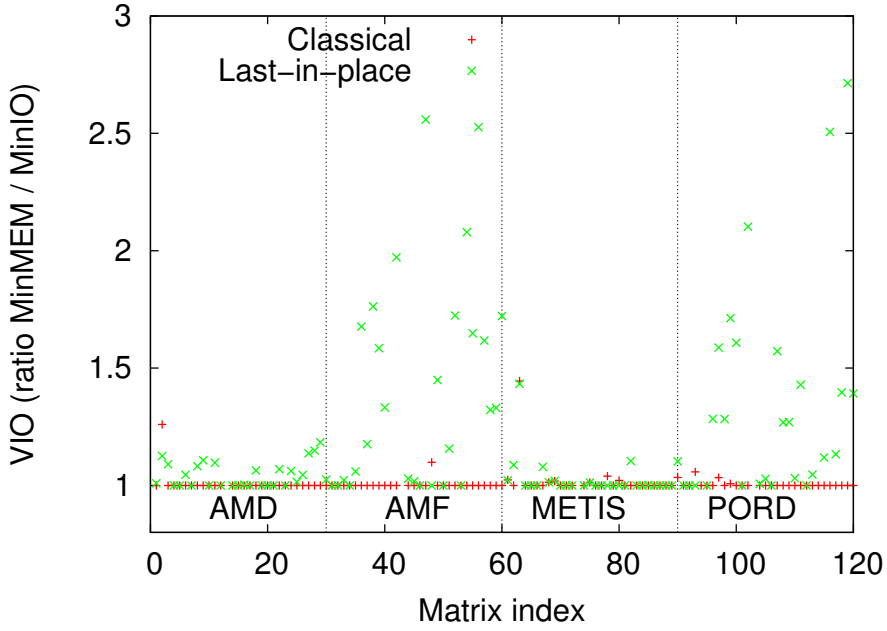
sequence $\rightarrow$ b-a-c

$A_{fath} = 14,\ V^{I/O} = 7$



Experimental Results: MinMEM vs MinIO

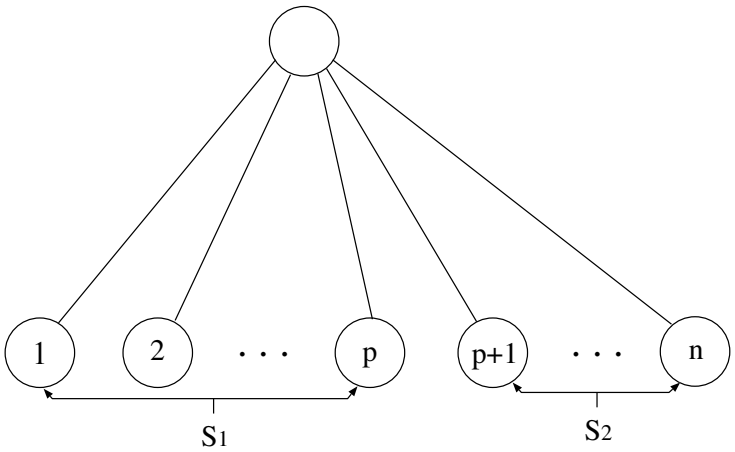




Volume decreased up to 50% in comparison to Liu's algorithm.

Outline

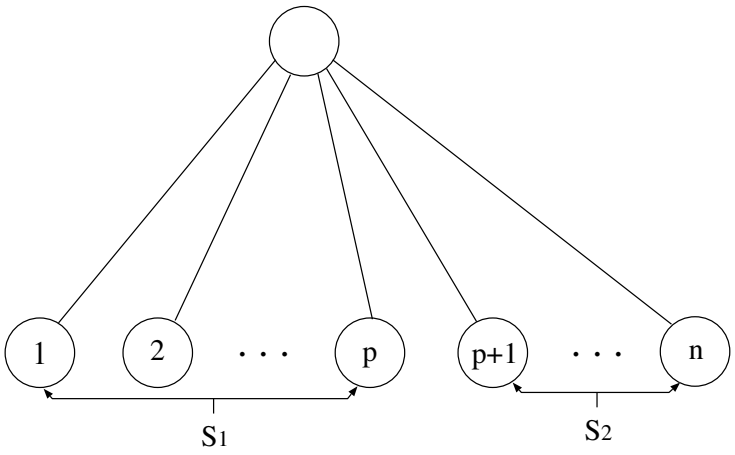
Flexible allocation scheme and I/O volume



- p is the position of the allocation of the parent
- $\mathcal{S}_1$ is the set of children treated before the allocation of the parent
- $\mathcal{S}_2$ is the set of children treated after the allocation of the parent

- Inside $\mathcal{S}_1$: behavior of the classical multifrontal scheme
- Inside $\mathcal{S}_2$: no impact of the order on the *I/O* volume
- We may write (partially/entirely) the parent at any time after its allocation provided we read it again as soon as a CB is produced

Flexible allocation scheme and I/O volume



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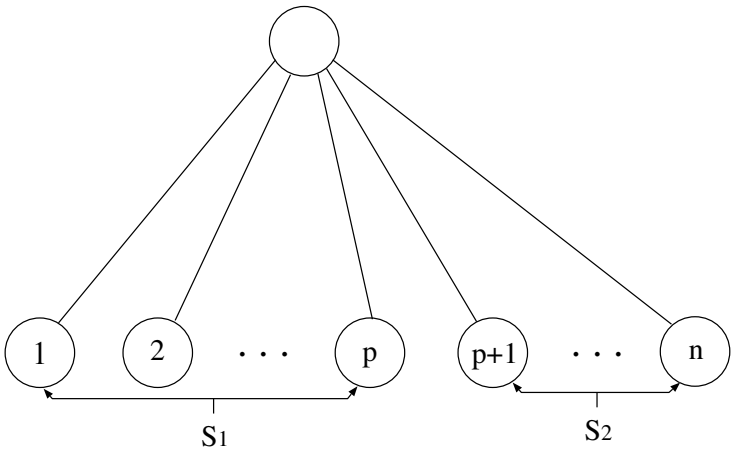

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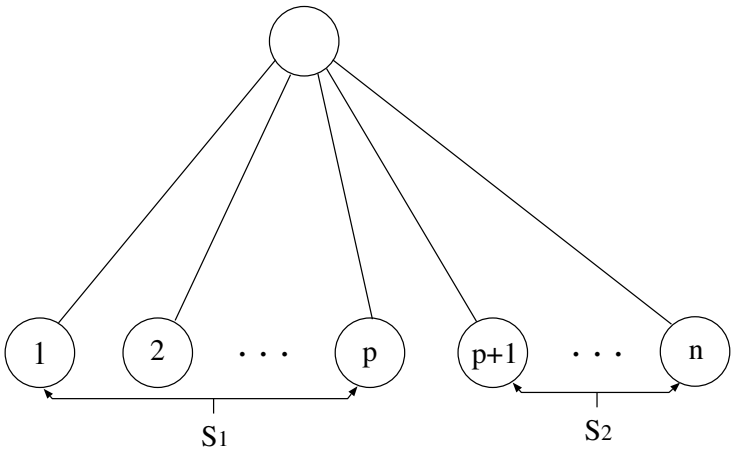
Flexible allocation scheme and I/O volume



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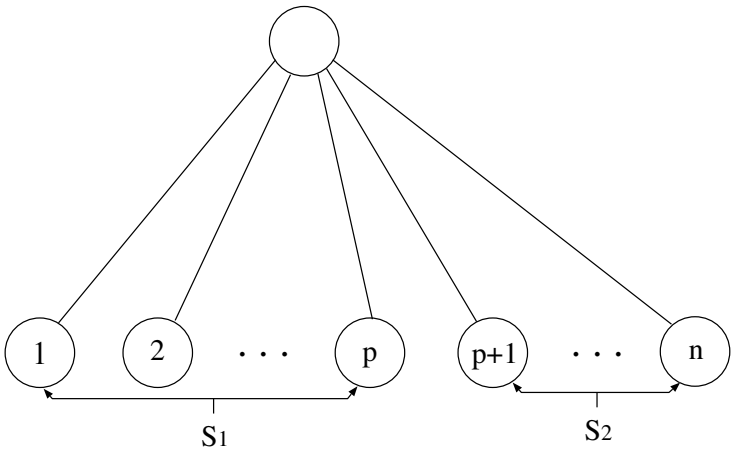

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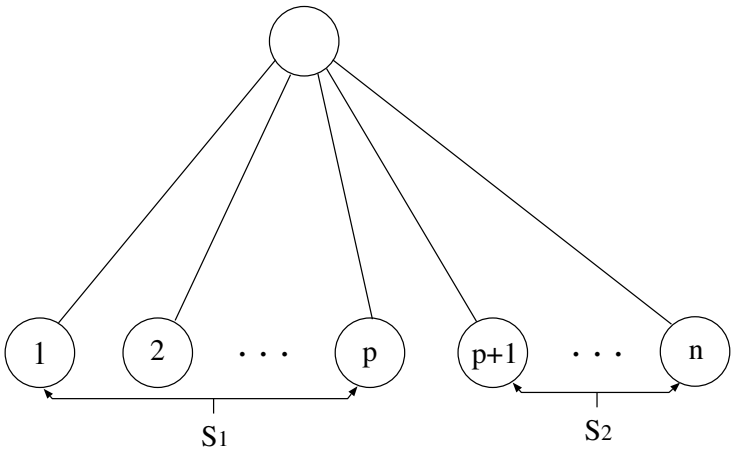
Flexible allocation scheme and I/O volume



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$$+ \sum_{i=1}^{n} V_i^{I/O}$$

Minimizing the I/O volume

Problem

1. In which order should we process the n children;
2. At which position p should we allocate the frontal matrix of the parent?

to minimize V_{family} on a given family ?

Complexity

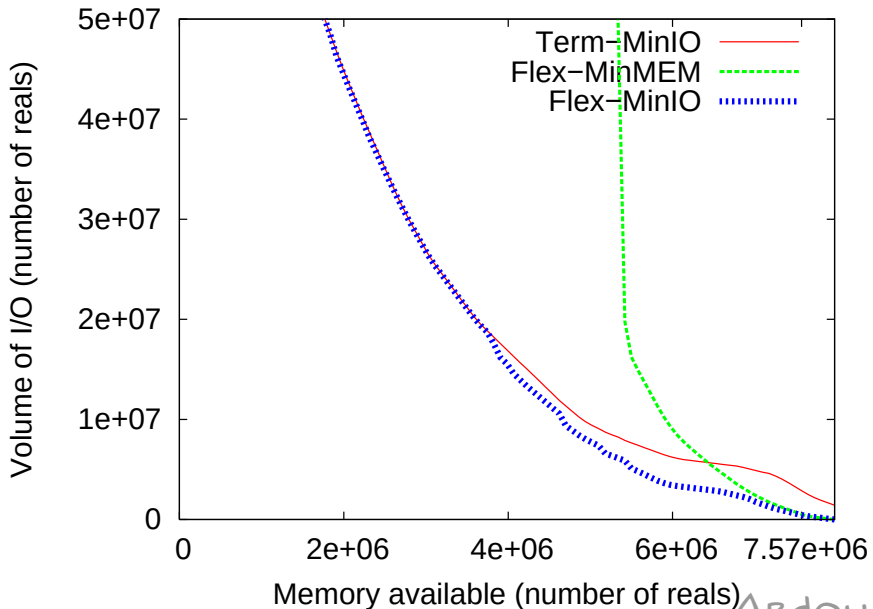
- Number of possibilities: $n \cdot n!$.
- Reduced to 2^n (2-partition):
  - order before allocation $\rightarrow$ our optimal algorithm;
  - order after allocation $\rightarrow$ does not matter.
- Cannot do "better" in general:
  - Problem NP-hard;
  - Proof: reduction from . . . 2-partition.

Heuristic

Algorithm.

All the children are initially in $\mathcal{S}_1$
repeat
move to $\mathcal{S}_2$ the child which is responsible for the peak of storage
until we cannot save anything

Results with the `TWOTONE` matrix ordered with `PORD`:



Outline

Conclusion and Future work

Memory

- New memory management schemes and corresponding memory minimization algorithms proposed.
- Active memory and total memory cases considered.

Volume of *I/O*

- Optimality for memory minimization $\not\Leftrightarrow$ optimality for volume of *I/O* minimization.
- Several contexts studied and various algorithms/heuristics proposed.

Future work:

- Real-life implementation (modification of the factorization).
- What about parallel executions?

Projet de recherche au sein de ROMA

Complexité croissante des plates-formes actuelles :

- Nécessité de s'adapter à l'hétérogénéité et à l'aspect grande échelle des plates-formes.
- Prise en compte de phénomènes de pannes et de consommation d'énergie.

Projet au sein de ROMA :

Algorithmique en lien avec le matériel et les architectures émergentes

- Exploitation des architectures multi-cœurs modernes.
- Utilisation des GPU et autres accélérateurs.
- Consommation d'énergie.
- Intégration des résultats de recherche dans des applications (MUMPS).