I/O-Efficient Algorithms and Data Structures

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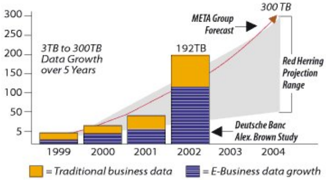
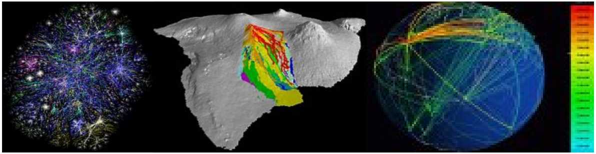
Large Data Sets

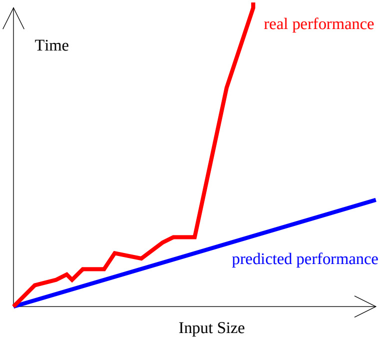
Sources of very large data volumes

- Data warehouses: enterprise data collections
- Geographic information systems: GoogleEarth, NASA's World Wind
- Computer graphics: visualize huge scenes
- Billing systems: phone calls, traffic
- Analyze huge networks: Internet, phone call graph
- Text collections: Google, YAHOO!, Ask.com, etc.





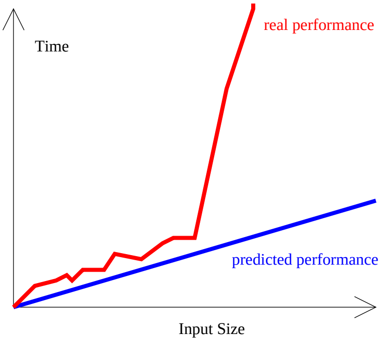
Scalability of Algorithms



How to process them

- Buy a TByte main memory? $\rightsquigarrow$ expensive or impossible
- Here: how to process very large data sets cost-efficiently

Scalability of Algorithms



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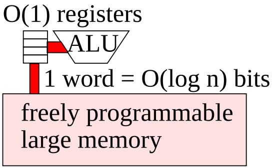
von Neumann RAM Model



In first year course:

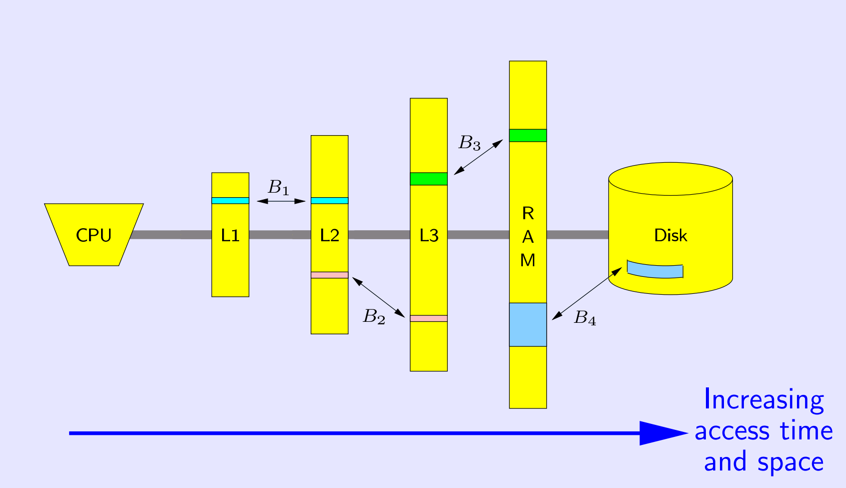
- Computer $\approx$ CPU $+$ Memory
- Uniform cost model:
  each access and each operation cost one unit of time

Impact:

- Very simple analysis
- Good estimation for first computers

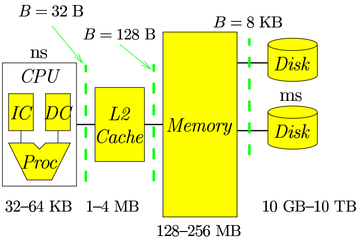
BUT: Modern computers have a deep HIERARCHY of memory

Modern Computer



Why Memory Hierarchies?

- Why: purely economic reasons !!!
- faster $\sim$ more expensive $\longrightarrow$ as few expensive pieces as possible.



	Latency	Relative to CPU
Register	0.5 ns	1
L1 cache	0.5 ns	1-2
L2 cache	3 ns	2-7
DRAM	150 ns	80-200
TLB	500+ ns	200-2000
Disk	10 ms	10^7

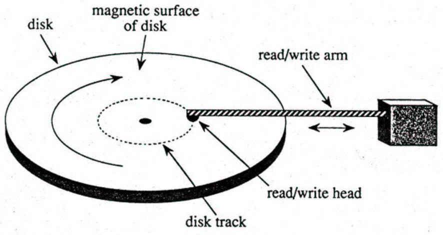
- Hard disks can be the ultimate performance killers.

Trends

Parameter	Yearly Improvement Rate
Disk Latency	10 %
Disk Bandwidth	20 %
Processor Speed	55 %
RAM Bandwidth	40 %
RAM Capacity/Cost	45 %

- Performance gap is increasing.
- RAM Capacity doubling about every two years but users doubling data storage about every 5 months (frequently copying everything).
- Results in I/O Bottleneck.

Why are Hard Disks such slow?



Components of disk access time:

- Seek time (milliseconds, SLOW)
- Rotational latency (milliseconds, SLOW)
- Read/write access (nanoseconds, FAST): bandwidth 40–80 MByte/s

> Reading many consecutive data items takes not much longer than reading a single data item
> $\Rightarrow$ balance seek time/rot. latency with bandwidth
> $\Rightarrow$ block size $\approx$ track size $\approx$ a few MBytes

How the Operation System tries to make up for it

Virtual Memory provides the look of the uniform model.

But not necessarily the performance !!!

Additionally:

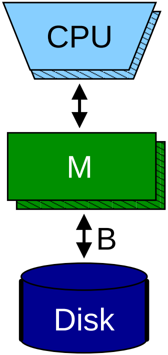
- Disk partitioned into blocks of $\geq$ 512 Bytes.
- Every disk access reads or writes a whole block.
- Read ahead.

This helps in special cases (e.g. scanning).

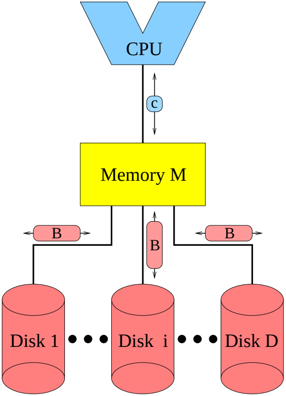
For most interesting algorithms this does not help at all.

Aggarwal–Vitter I/O model

- N — size of input
- M — size of main memory ($M \ll N$)
- B — size of transfer block (128KB .. 2 MB)
- Cost measure – number of I/Os
- I/O-efficient alg. $\equiv$ External memory alg. $\equiv$ Secondary memory alg.



Parallel Disk Model [VitterShriver]



- Main memory size $M \ll$ Problem size N
- External memory = D disks
- Data is transfered in blocks of size B
- Up to $\leq D \cdot B$ data per I/O step (10^2 per sec.)
- Goal 1: Minimize number of I/O steps
- Goal 2: Minimize number of CPU instructions
- $\text{scan}(x) := \Theta(\frac{x}{D \cdot B})$ I/Os.
- $\text{sort}(x) := \Theta(\frac{x}{D \cdot B} \cdot \log_{M/B} \frac{x}{B})$ I/Os.

How to make algorithms I/O-efficient?

Only a few golden rules:

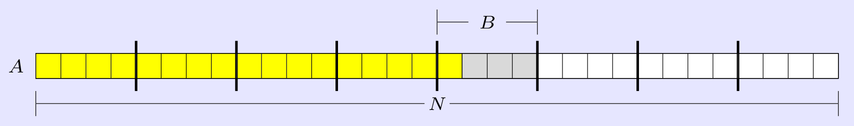
- Avoid unstructured access patterns.
- Incorporate LOCALITY directly into the algorithm.

Tools:

- Scanning: $\mathrm{scan}(N) = O\left(\frac{N}{DB}\right)$ I/Os.
- Sorting: $\mathrm{sort}(N) = O\left(\frac{N}{DB}\left\lceil\log_{M/B}\frac{N}{M}\right\rceil\right)$, usually $\left\lceil\log_{M/B}\frac{N}{M}\right\rceil = 2$.
- Special I/O-efficient data structures.
- “Simulation” of parallel algorithms.

Warmup: Scanning

```
sum = 0;
for i=1 to N do sum := sum + A[i];
```



$scan(N) = O(N/B)$ I/Os, optimal.

Sorting: THE tool for Reordering

Importance of Sorting - An Example

```
int[1..N] A,B,C;
for i=1 to N do A[i]:=B[C[i]];
```

$\Rightarrow$ Worst case: $\Omega(N)$ I/Os. $N = 10^6$, $T = 10000$ sec $\approx$ 3 hours

Better:

```
SCAN C:     (C[1]=17,1),  (C[2]=5,2),   ...
SORT(1st):  (C[73]=1,73), (C[12]=2,12), ...
par SCAN :  (B[1],73),    (B[2],12),    ...
SORT(2nd):  (B[C[1]],1),  (B[C[2]],2),  ...
```

$\Rightarrow$ Worst case: $\text{sort}(N) \approx O(N/DB)$ I/Os. $B = 100KBytes$, $T < 1$ sec.

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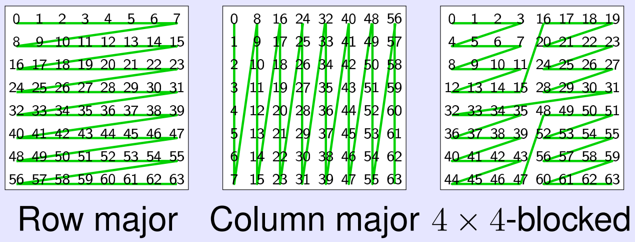
Matrix Transposition

Problem:

$$C = A^T \ , \ C_{i,j} = A_{j,i}$$

Layout of matrices:



Matrix Transposition: Algorithm1

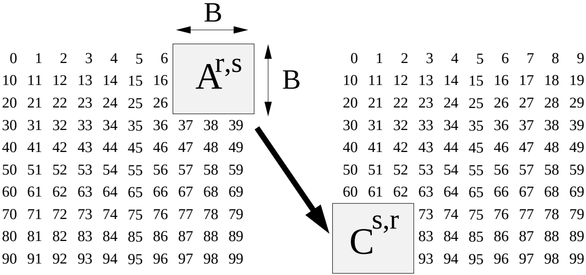
Algorithm 1: Nested loops

```
for (i=0; i<N; i++)
  for (j=0; j<N; j++)
    C[j][i] = A[i][j];
```

- Row major
- Writing a column of $C \Rightarrow \Theta(N)$ I/Os
- Total $O(N^2)$ I/Os

Matrix Transposition: Algorithm2

Algorithm 2: **Blocked** algorithm



- Partition A (C) into submatrices $A^{r,s}$ ($C^{r,s}$) of size $B \times B$, $B^2 = \Theta(M)$.
- Transfer each submatrix $A^{r,s}$ to the internal memory $\Rightarrow B$ I/Os
- Apply Algorithm 1 to $A^{r,s}$ (internally)
- Transfer it to $C^{s,r} \Rightarrow B$ I/Os

$2\frac{N^2}{B^2} \cdot B = O\left(\frac{N^2}{B}\right)$ I/Os, optimal.

Matrix Multiplication

Problem:

$$Z = X \cdot Y,\ z_{ij} = \sum_{k=1}^{N} x_{ik} \cdot y_{kj}$$

Matrix Multiplication

Algorithm 1: Nested loops

- Row major
- Reading a column of $Y \Rightarrow N$ I/Os
- Total $O(N^3)$ I/Os

$$
\begin{array}{l}
\text{for } i = 1 \text{ to } N \\
\quad \text{for } j = 1 \text{ to } N \\
\qquad z_{ij} = 0 \\
\qquad \text{for } k = 1 \text{ to } N \\
\qquad\quad z_{ij} = z_{ij} + x_{ik} \cdot y_{kj}
\end{array}
$$

Algorithm 2: Blocked algorithm

- Partition X and Y into blocks of size $s \times s$, $s = \Theta(\sqrt{M})$.
- Apply Algorithm 1 to $N/s \times N/s$ matrices; elements are $s \times s$ sub-matrices.
- Use $s \times s$-blocked layout.

$\mathcal{O}((N/s)^3 \cdot s^2/B) = \mathcal{O}(N^3/(s \cdot B)) = \mathcal{O}(N^3/(B \cdot \sqrt{M}))$ I/Os, optimal.

Matrix Multiplication

Algorithm 1: Nested loops

- Row major
- Reading a column of $Y \Rightarrow N$ I/Os
- Total $O(N^3)$ I/Os

```
for i = 1 to N
    for j = 1 to N
        z_ij = 0
        for k = 1 to N
            z_ij = z_ij + x_ik · y_kj
```

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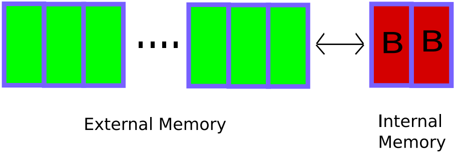
Simple I/O-Efficient Data Structures

Stack (LIFO Order – Last In First Out):

- Maintain an combined input/output buffer of size $2 \cdot B$ in memory.
- Push: Insert new element into buffer;
  if buffer now full, write **bottom B elements** to disk.
- Pop: remove top element from buffer;
  if buffer now empty, read next block from disk.

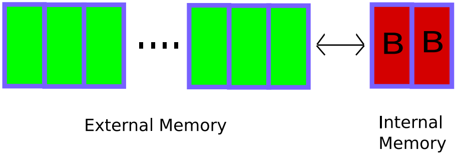
I/O-complexity of Push/Pop:

- Best-Case: 0 I/Os
- Worst-Case: 1 I/O
- Amortized: $1/B$ I/Os



Obs: After an I/O, the buffer contains exactly B elements.

I/O-Efficient Stack



Question: Why do need TWO blocks in internal memory?

FIFO-Queue

First In First Out Queue

- Maintain an **input buffer** and an **output buffer** (each of size B) in memory.
- Insert: put new element into input buffer;
  if buffer now full, write to disk.
- Remove: take element from output buffer (if empyt from imput buffer);
  if buffer now empty, read next block from disk.

I/O-complexity of Insert/Remove:

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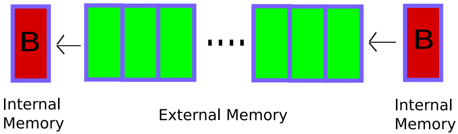
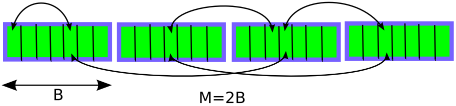


Lists

- Direct implementation: 1 I/O for when following a link, $\Theta(N)$ I/Os for traversing N elements

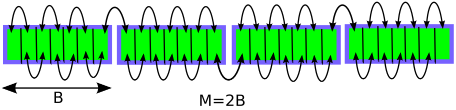


- Faster $O(\mathrm{sort}(N))$ traversal: list ranking preprocessing, later

Lists cont.

First attempt:

- Use locality: store *B* consecutive elements together



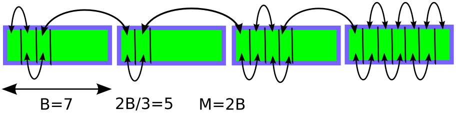
$\Rightarrow$ Traversal: $N/B = O(\text{scan}(N))$ I/Os 

- An insertion or deletion can cost $\Theta(N/B)$ I/Os 

Lists cont. 2

Second attempt:

- Relax the invariant: $\geq \frac{2}{3}B$ elements in every pair of consecutive blocks



- Traversal: $\leq 3N/B = O(\mathrm{scan}(N))$ I/Os
- Insertion into block i:
  - block i is space: 1 I/O
  - block i is full:
    - a neighbor has space: push an element to it, $O(1)$ I/Os
    - both neighbors are full: split block i into 2 blocks of $\approx B/2$ elements, $O(1)$ I/Os ($\geq B/6$ deletions needed to violate the invariant)
  - Deletion from block i:
    if blocks i and $i+1$ or blocks i and $i-1$ have $\leq 2B/3$ elements
    $\Rightarrow$ merge the two blocks, $O(1)$ I/Os

$\Rightarrow$ $O(1)$ I/Os per update (the best for lists)

The STXXL Library

I/O-Efficient Software Libraries

Advantages

- Abstract away the technical details of I/O
- Provide implementation of basic I/O-eff. algorithms and data structures

⇒ Boost algorithm engineering

Existing Libraries

- TPIE: many (geometric) search data structures
- LEDA-SM: extension of LEDA (discontinued)

+ Good demonstrations of the external memory concepts

– Do not implement many features that speed up I/O-efficient algorithms

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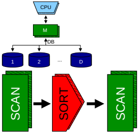
The STXXL Library

- STL – C++ Standard Template Library, implements basic containers (maps, sets, priority queues, etc.) and algorithms (quicksort, mergesort, selection, etc.)
- STXXL : Standard Template Library for XXL Data Sets

  `http://stxxl.sourceforge.net`

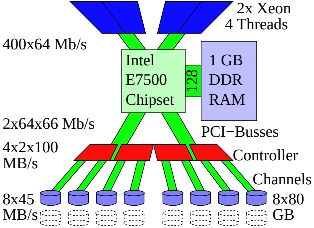
  containers and algorithms that can process huge volumes of data that only fit on disks (I/O-efficient)
  - Compatible with STL
  - Performance–oriented

STXXL Features



- Transparent parallel disk support
- Handles very large problems (up to petabytes)
- Pipelining saves many I/Os
- Explicitly overlaps I/O and computation
- Avoids superfluous copying
  - in OS I/O subsystem and the library itself
- Compatible with STL – C++ Standard Template Library
  - Short development times
  - Reuse of STL code (e.g. selection alg.)

Engineering Parallel Disk Systems



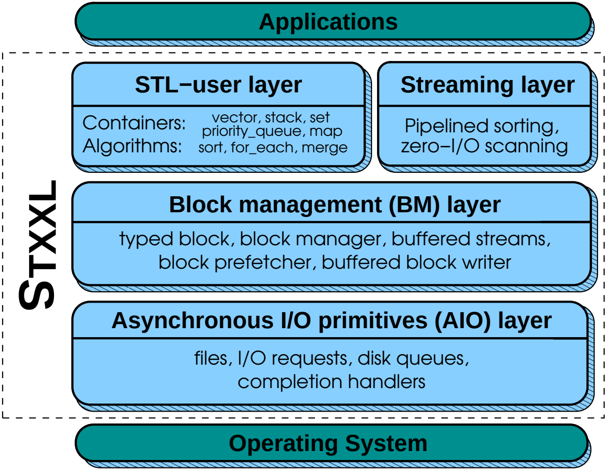
Challenges

- Cheap case for $\geq$ 8 hard disks
- Many fast PCI slots for ATA controllers (no bus bottlenecks)
- Wide Parallel ATA cables worsen airflow (later system use Serial ATA)
- File system scalability: very large files

$\Rightarrow$ 375 MB/s ($\approx$ 98% of the peak) for about 3000 Euro in 2002

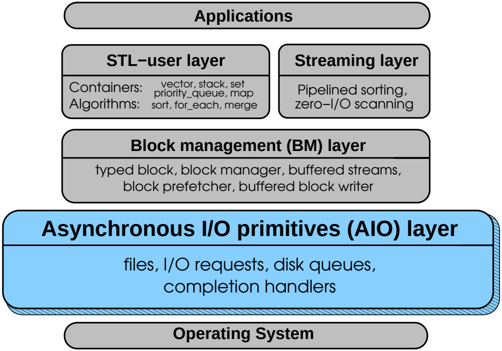
$\Rightarrow$ Other systems: 10 disks $=$ 640 MB/s, 4 disks $=$ 214 MB/s

STXXL Design



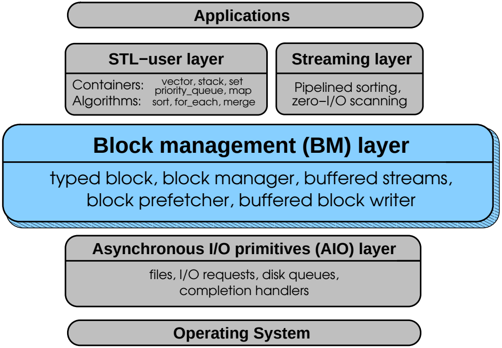
STXXL Design: AIO Layer

- Hides details of async. I/O (portability, user-friendly)
- Implementations for Linux/MacOSX/BSD/Solaris and Windows systems
- Asynchrony provided by POSIX threads or Boost Threads
- Unbuffered I/O support: more control over I/O



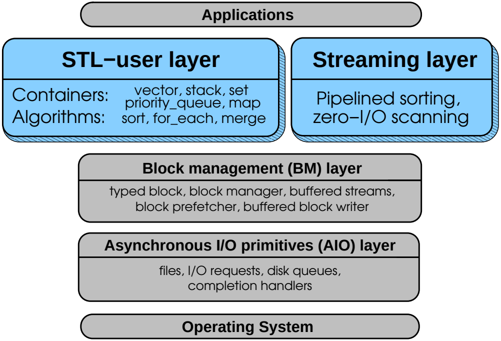
STXXL Design: BM Layer

- Block abstraction
- Parallel disk model
- (Randomized) striping and cycling
- Parallel disk buffered writing and optimal prefetching [Hutchinson&Sanders&Vitter01]



STXXL User Layers

- STL-user layer: compatible with STL, vector, stack, queue, deque, priority queue, map, sorting, scanning
- Streaming layer: programming with pipelining



Some STXXL Containers

Stacks:

- Few variants
  - Classic, has 2 blocks
  - Grow-shrink, does prefetching/buffering (own buffer pool)
  - Grow-shrink 2, does prefetching/buffering (shared buffer pool)

Queue:

- the same buffering techniques as `stxxl::stack`

Vector – ST(XX)L dynamic array:

- caches some blocks (LRU)
- $O(N/DB)$ I/Os scanning

Deque: double ended queue

- push/pop from/to the both ends in $O(1/DB)$ I/Os
- implemented as adapter of `stxxl::vector` (circular wrapping)

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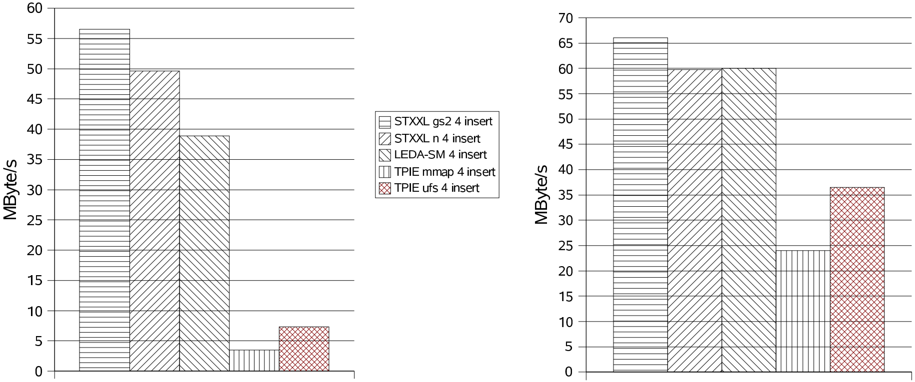
Experiments with Stacks: Insertion

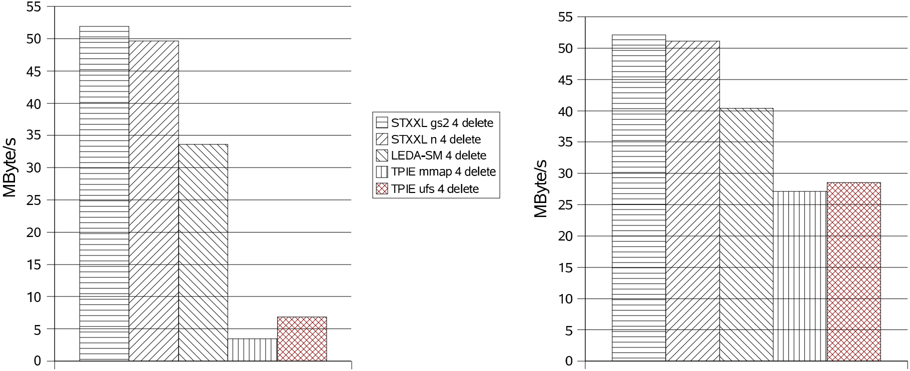
gs2=grow-shrink (overlapping) stacks n=normal/classic stacks (2B buffer)



4-byte elements 32-byte elements

Experiments with Stacks: Deletion

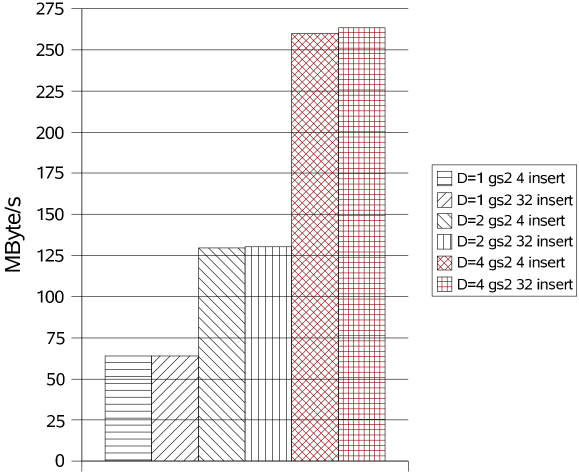
gs2=grow-shrink (overlapping) stacks n=normal/classic stacks ($2B$ buffer)



4-byte elements   32-byte elements

Experiments with Stacks: Multiple Disks Insertion

gs2=grow-shrink (overlapping) stacks



4/32-byte elements

Some STXXL containers

Map (search tree):

- implemented as B$^+$-tree, later
- caches some nodes and leaves in internal memory (LRU)
- $O(\log_B N)$ I/Os for LOCATE query
- supports iterators: $O(N/B)$ I/Os for range scanning

Priority queue:

- implemented as sequence heap, later
- non-addressable
- $\approx O\left(\frac{1}{N}\mathrm{sort}(N)\right)$ I/Os for DELETEMIN, INSERT
- overlapping, prefetching, buffering

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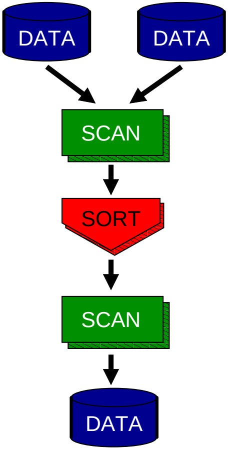
- non-addressable
- $\approx O\left(\frac{1}{N}\mathrm{sort}(N)\right)$ I/Os for DELETEMIN, INSERT
- overlapping, prefetching, buffering

Generate Random Graph with STXXL

```
stxxl::vector<edge> Edges(10000000000ULL);
std::generate(Edges.begin(),Edges.end(),random_edge());
stxxl::sort(Edges.begin(),Edges.end(),edge_cmp(),
                              512*1024*1024);
stxxl::vector<edge>::iterator NewEnd =
                              std::unique(Edges.begin(),Edges.end());
Edges.resize(NewEnd - Edges.begin());
```

Streaming Layer and Pipelining

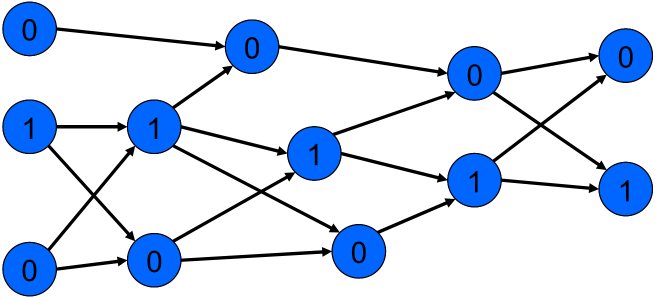


- EM algorithm ⇒ data flow through a DAG
- Feed output data stream directly to the consumer algorithm
- A new iterator-like interface for EM algorithms
- Basic pipelined implementations (file, sorting nodes, etc.) provided by STXXL
- Saves many I/Os (factor 2–3) in many EM algorithms

STXXL Performance: a Benchmark

- Maximal Independent Set (+input generation)
  - An independent set *I* is a set of nodes on a graph *G* such that no edge in *G* joins two nodes in *I*. A maximal independent set is an independent set such that adding any other node would cause the set not to be independent anymore.
- I/O optimal algorithm [ZehPhd]: time-forward processing, scanning, sorting, priority queue

Time-Forward Processing: Evaluating a Directed Acyclic Graph



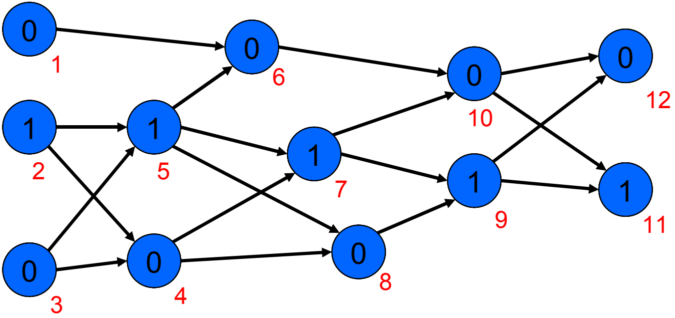
Given a labelling ϕ, compute a labelling ψ so that $\psi(v)$ is computed from $\phi(v)$ and $\psi(u_1), \ldots, \psi(u_r)$, where $u_1, \ldots, u_r$ are v's in-neighbors.

Time-Forward Processing

- Assume nodes are given in topologically sorted order.

⇒ Use priority queue Q to send data along the edges.

- Node ID ≡ PQ priority
- Send message x from u to v ≡ INSERT(v,x)
- Receive message x at node v ≡ (v,x):=DELETEMIN()



Time-Forward Processing

Analysis:

- Vertex set + adjacency lists scanned

$\Rightarrow$ $O(\text{scan}(|V|+|E|))$ I/Os

- Priority queue:
  - Every edge inserted into and deleted from Q exactly once

  $\Rightarrow$ $O(|E|)$ priority queue operations (each costs $O\left(\frac{1}{|E|}\text{sort}(|E|)\right)$ I/Os)

$\Rightarrow$ Total: $O(\text{sort}(|E|))$ I/Os

MIS: Pseudocode

GreedyMIS:

```
I := 0
for every vertex v in G do
  if no neighbor of v is in I then
     Add v to I
  end if
end for
```

MIS: STXXL Code

`edges`: sorted outgoing edges (adjacency lists)

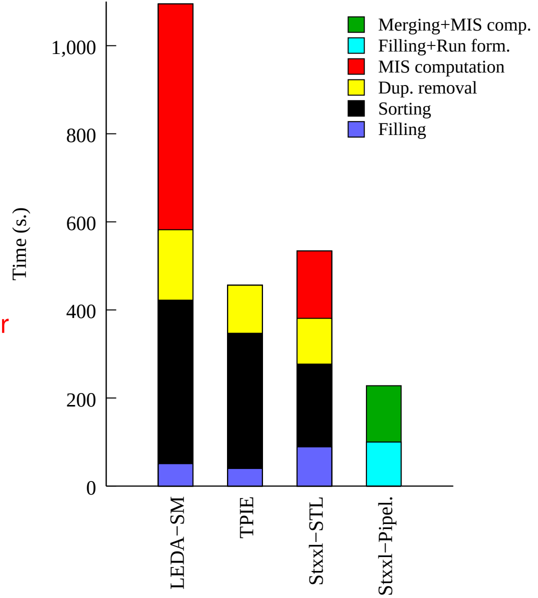
`depend`: event queue

v $\in$ `depend` if $\exists\, u$: $(u, v) \in E \wedge u \in$MIS (i.e. v cannot be included into MIS)

```
pq_type depend(PQ_PPOOL_MEM,PQ_WPOOL_MEM);
stxxl::vector<node_type> MIS; // output
for (;!edges.empty();++edges) {
        while (!depend.empty() && edges->src > depend.top())
                depend.pop(); // delete old events
        if (depend.empty() || edges->src != depend.top() ) {
                if (MIS.empty() || MIS.back() != edges->src )
                        MIS.push_back(edges->src);
                depend.push(edges->dst);
        }
}
```

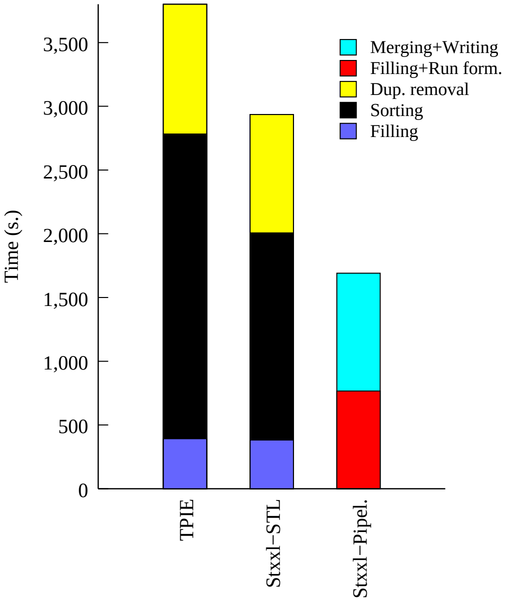
MIS: Running Times

- Debian Linux, `g++ -O3`
- 2×Xeon 2GHz
- single disk
- N = 2000 MBytes
- M = 512 MBytes
- TPIE: only graph gen.
- STXXL PQ is 3 times faster



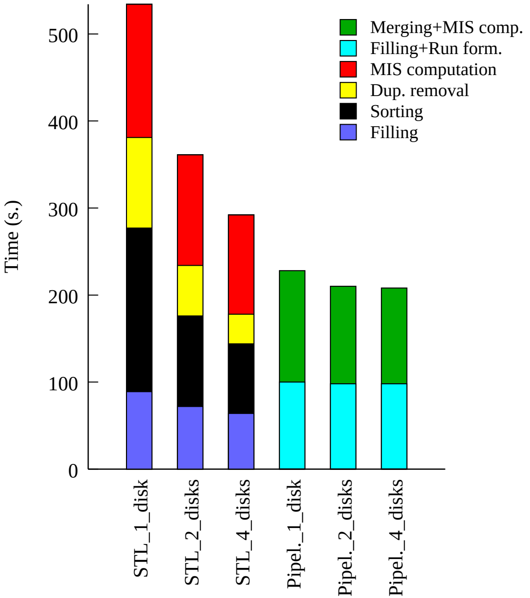
MIS: Larger Inputs

- Only graph generation
- single disk
- N = 16 GBytes
- M = 512 MBytes
- Scales well



MIS: More Disks

- 2,4 disks
- N = 2000 MBytes
- M = 512 MBytes
- Pipel. – CPU bound
- I/O-wait counters



MIS: The Largest Graph

- The largest graph:
- $4.3 \cdot 10^9$ nodes, $13.4 \cdot 10^9$ edges = 100 GBytes
- Working space takes 4 hard disks
- Computation on an Opteron system took 3h 7min

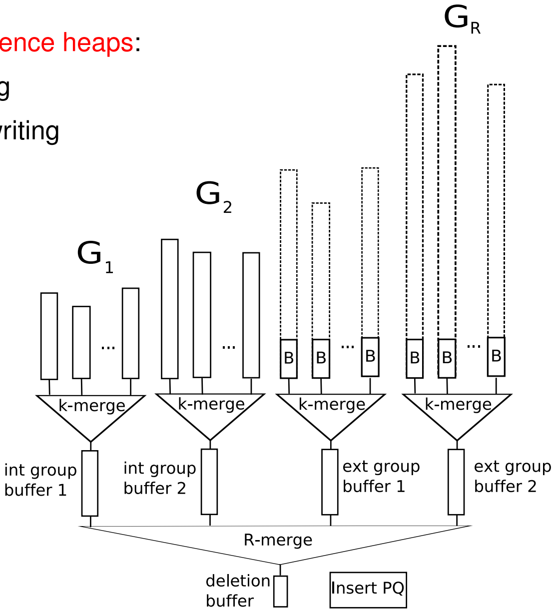
Active STXXL Users We Know About

1. University of Karlsruhe, Germany (text processing, graph algorithms, practical courses)
2. Max-Planck-Institut für Informatik, Germany (bio-informatics, graph algorithms)
3. DIMACS Center, Rutgers University, USA (graph analysis, data mining)
4. University of Rome “La Sapienza”, Italy (connected components)
5. University of Texas at Austin, USA (Gaussian elimination)
6. Bitplane AG, Switzerland (visualization and analysis of 3D and 4D microscopic images)
7. Philips Research, The Netherlands (differential cryptographic analysis)
8. Dalhousie University, Canada (N-gram extraction)
9. Florida State University, USA (construction of Voronoi diagrams)
10. Montefiore Institute, Belgium (big sparse matrices)
11. University of British Columbia, Canada (topology analysis of large networks)
12. Bayes Forecast, Spain (statistics and time series analysis)
13. Indian Institute of Science in Bangalore, India (suffix array construction)
14. Rensselaer Polytechnic University, USA (suffix array construction)
15. Institut français du pèrole, France (analysis of seismic files)
16. Northumbria University, UK (search trees)
17. University of Trento, Italy (text compression)
18. Norwegian University of Science and Technology in Trondheim, Norway (suffix array construction)

STXXL Priority queue

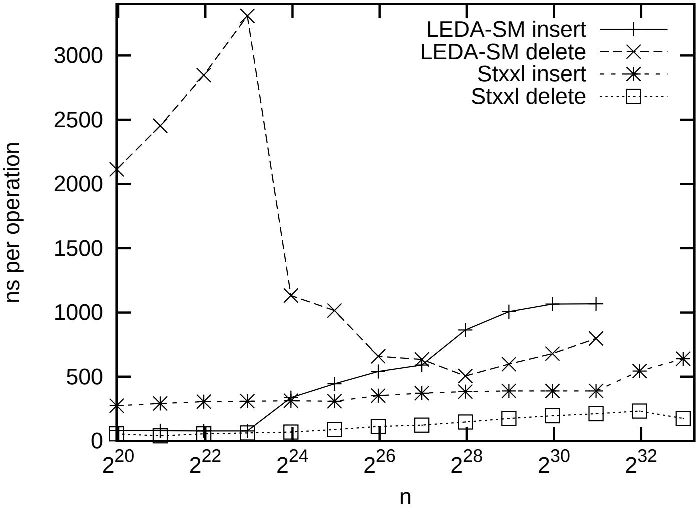
Based on sequence heaps:

- + prefetching
- + buffered writing

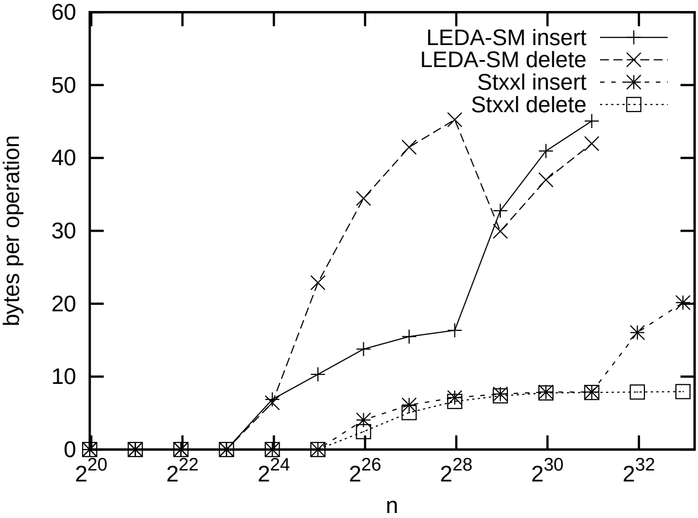


Insert-All-Delete-All Time

3 Ghz Pentium 4, $M = 1$ GByte, 1 SATA disk, random input



Insert-All-Delete-All I/O Volume



I/O-volume 2 – 5.5 times less than [Brengel at al.](LEDA-SM) !

Searching I/O-efficiently

In internal memory:

- `std::binary_search` (static search)
- `std::map` (dynamic binary red-black tree)

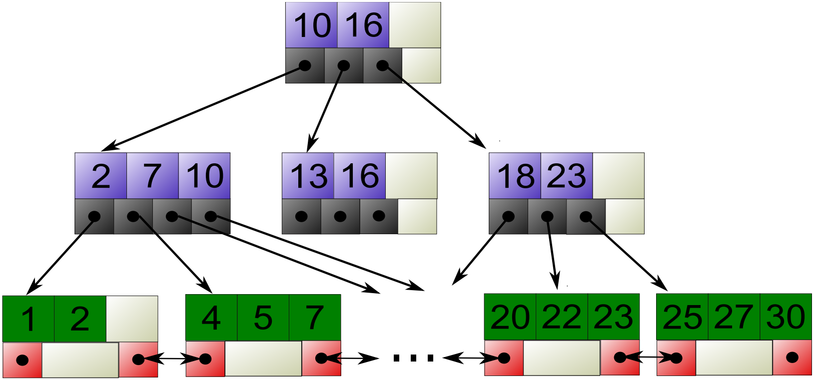
$\Rightarrow$ I/O-inefficient $O(\log_2 N)$ I/Os

Implement STXXL searching (`stxxl::map`) as a B^+-tree

Searching I/O-efficiently cont.

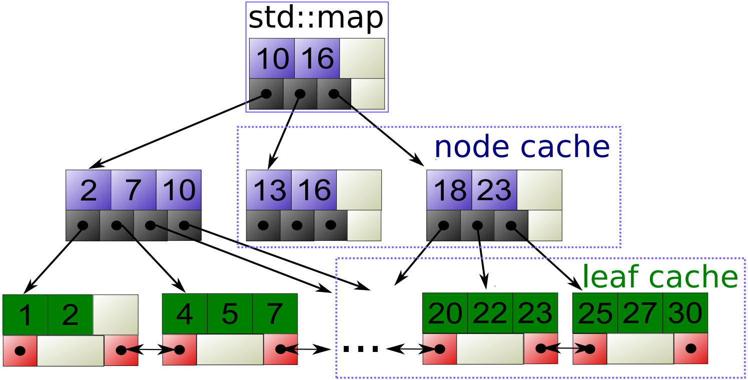
Implement STXXL searching (`stxxl::map`) as a B^+-tree:

- generalization of binary trees: up to B children per node
- $O(\log_B N)$ I/Os for LOCATE, INSERT, DELETE
- very practical: used in relational databases, NTFS, ReiserFS, XFS, ...



Implementation of `stxxl::map`

- **root** as `std::map` with size limit
- LRU cache for internal nodes
- LRU cache for leaves
- full support of STL iterators, N/B I/O scanning with prefetching



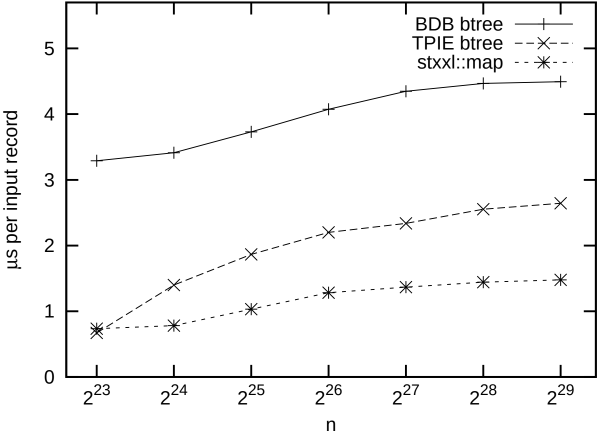
Experiments with `stxxl::map`

Dual-Core Opteron 2GHz, M=1GByte, D=1

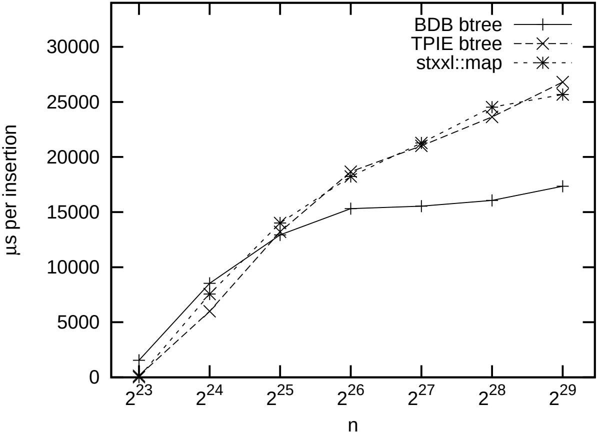
32-bit random keys, 32-bit data field

Competitors: TPIE, Berkeley DB (used e.g. in MySQL)

Bulk construction:



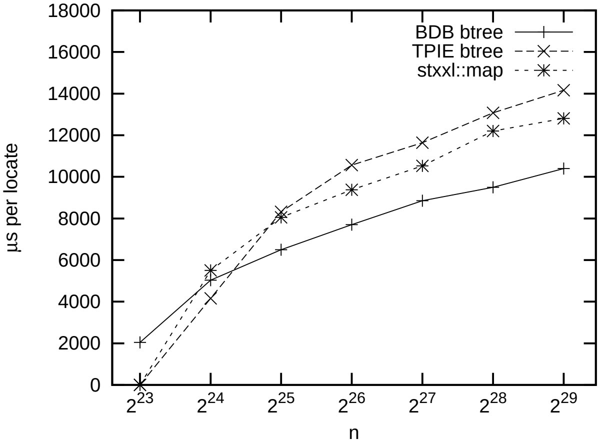
Insert 100.000 random records



100 % fill factor: load 2 leaves and save 3 leaves per insertion = 25 ms

BDB compresses key prefixes, less I/Os, tuned splitting heuristics

Locate 100.000 random records



load random leaf = 10-13 ms

Berkeley DB Interfaces

```
struct my_key { char keybuf[KEY_SIZE]; };
struct my_data { char databuf[DATA_SIZE]; };

Dbc *cursorp; // data base cursor
// db is the BDB B-tree object
db.cursor(NULL, &cursorp, 0); // initialize cursor

for (int64 i = 0; i < n_locates; ++i)
{
  rand_key(key_storage); // generate random key
  // initialize BDB key object for storing the result key
  Dbt keyx(key_storage.keybuf,KEY_SIZE);
  // initialize BDB key object for storing the result data
  Dbt datax(data_storage.databuf,DATA_SIZE);
  cursorp->get(&keyx, &datax,DB_SET_RANGE); // perform locate
}
```

C-like, no templates

STXXL Interfaces

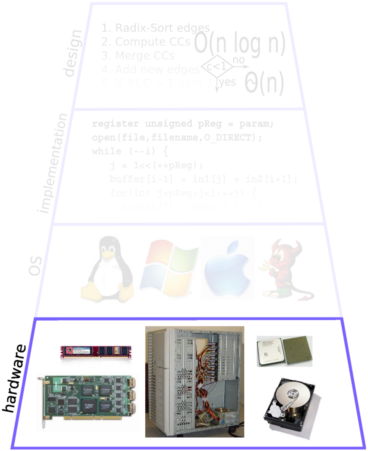
```
struct my_key { char keybuf[KEY_SIZE]; };
struct my_data { char databuf[DATA_SIZE]; };

std::pair<my_key,my_data> element; // key—data pair

for (i = 0; i < n_locates; ++i)
{
  rand_key(i,element.first); // generate random key

  // perform locate, CMap is a constant reference to a map object
  map_type::const_iterator result = CMap.lower_bound(element.first);
}
```

simple, stronger typing

Algorithm Engineering for Large Data Sets

Engineering from the bottom to the top:

- many disks ⇝ CPU-bound ⇝ look at internal algorithms, RAID-0 ⇝ suboptimal
- Pipelining to save I/Os, overlap I/O and computation, easy to use library, abstraction, rapid prototyping
- Controlled unbuffered asynchronous I/O, scalable file systems
- Bottleneck-free hardware I/O-subsystem with parallel disks



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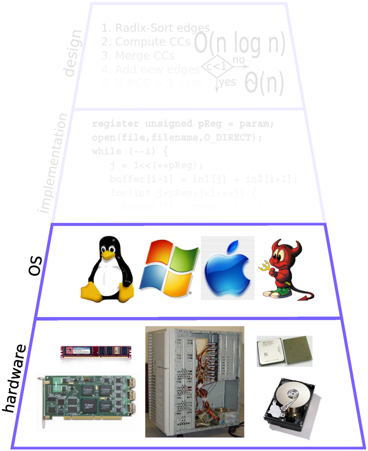

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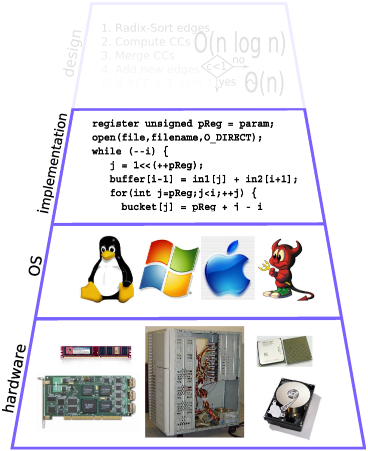

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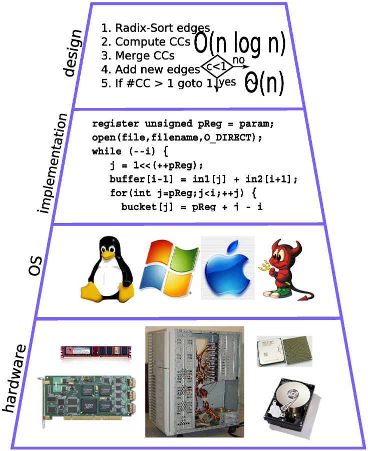


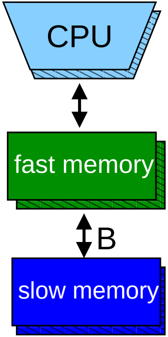
Some Cache Configurations

Only a few systems:

	Pentium 4	Pentium III	MIPS 10000	AMD Athlon	Itanium 2
Clock rate	2400 MHz	800 MHz	175 MHz	1333 MHz	1137 MHz
L1 data cache size	8 KB	16 KB	32 KB	128 KB	32 KB
L1 line size	128 B	32 B	32 B	64 B	64 B
L1 associativity	4-way	4-way	2-way	2-way	4-way
L2 cache size	512 KB	256 KB	1024 KB	256 KB	256 KB
L2 line size	128 B	32 B	32 B	64 B	128 B
L2 associativity	8-way	4-way	2-way	8-way	8-way
TLB entries	128	64	64	40	128
TLB associativity	full	4-way	64-way	4-way	full
RAM size	512 MB	256 MB	128 MB	512 MB	3072 MB

How can we write portable code that runs efficiently on different multilevel caching architectures?

Cache-Obliviousness



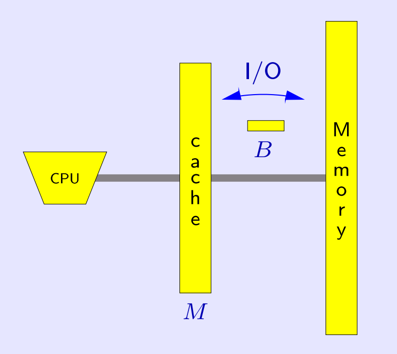
- N — size of input
- M — size of main/fast memory ($M \ll N$)
- B — size of transfer block
- Cost measure – number of I/Os

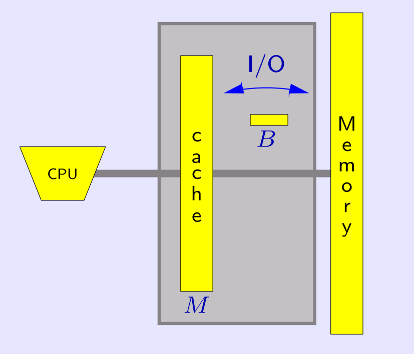
- Cache-Oblivious (CO) Model: M,B unknown to the algorithm

$\Rightarrow$ Good on one level $\Rightarrow$ good on all memory levels

$\Rightarrow$ One algorithm for all platforms ?!

Cache-Aware (I/O Model) vs. Cache-Oblivious





Cache-aware: fixed parameters *M* and *B*

Cache-oblivious: no parameters?! no tuning required ?!

Ideal-Cache Model

[Frigo, Leiserson, Prokop, Ramachandran 1999].

- Program with only **one** memory (single cache, hidden).
- Analysis like in I/O model; assumes arbitrary M and B.
- Suppose **optimal off-line cache replacement** strategy for M and B.
- Suppose **fully-associative cache**.

Realistic ??

- Multi-level.
- LRU (least recently used) replacement.
- Limited associativity.

Justification of the Ideal-Cache Model

Optimal replacement: LRU + 2$\times$ cache size $\Rightarrow$ at most 2$\times$ cache misses [ST85]

Corollary: If $T_{M,B}(N) = \mathcal{O}(T_{2M,B}(N))$ (**regularity condition**)
$\Rightarrow$ # cache misses using LRU is $\mathcal{O}(T_{M,B}(N))$.

Two memory levels: Optimal cache-obliv. alg. with $T_{M,B}(N) = O(T_{2M,B}(N))$
$\Rightarrow$ optimal # cache misses on each level of a multilevel LRU cache.

Fully-associative cache: Simulation of LRU (needs to know *M* and *B*)

- Direct mapped cache.
- Explicit memory management.
- Dictionary (2-universal hash functions) of cache lines in memory
- Expected $O(1)$ access time of cache line in memory.

How to make algorithms cache-oblivious?

Only a few golden rules:

- Avoid unstructured access patterns.
- Incorporate LOCALITY directly into the algorithm.

Tools:

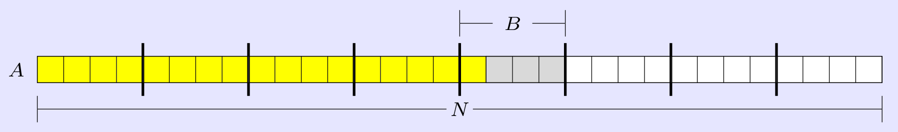
- Scanning.
- Sorting.
- Special cache-oblivious data structures and data layouts.
- "Simulation" of parallel algorithms.
- Divide and Conquer / Recursion
- Tall-Cache Assumption ($M = \Omega(B^2)$). $B = 16 - 128$ bytes!

Warmup: Scanning

already cache-oblivious!

```
sum = 0;
for i=1 to N do sum := sum + A[i];
```

$\text{scan}(N) = O(N/B)$ I/Os, optimal.



Remarks:

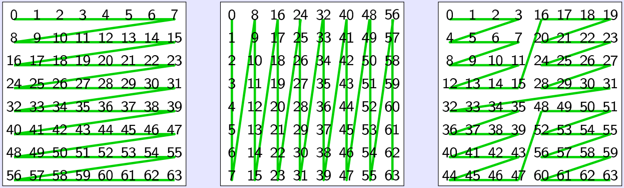
- No need to know B here.
- Scanning backwards would be slower in practice.

Repetition: Matrix Transposition

Problem:

$$C = A^T \;,\; C_{i,j} = A_{j,i}$$

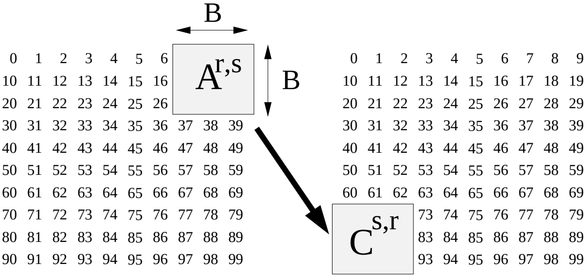
Layout of matrices:



Row major Column major 4×4-blocked

Repetition: Cache-Aware Matrix Transposition

Algorithm 2: **Blocked** algorithm



- Partition A (C) into submatrices $A^{r,s}$ ($C^{r,s}$) of size $B \times B$, $B^2 = \Theta(M)$.
- Transfer each submatrix $A^{r,s}$ to the internal memory $\Rightarrow$ B I/Os
- Apply Algorithm 1 to $A^{r,s}$ (internally)
- Transfer it to $C^{s,r}$ $\Rightarrow$ B I/Os

$2\frac{N^2}{B^2} \cdot B = O\left(\frac{N^2}{B}\right)$ I/Os, optimal.

CO Matrix Transposition

$$A = \begin{pmatrix} A1 & A2 \end{pmatrix} \quad C = \begin{pmatrix} C1 \\ C2 \end{pmatrix}$$

```
CO_Transpose(A,C)
{
    CO_Transpose(A1,C1);
    CO_Transpose(A2,C2);
}
```

I/O-complexity :

Case I: $N \leq \alpha B$ then $Q(N) \leq N^2/B + O(1)$ I/Os

Case II: $N > \alpha B$ then $Q(N) = 2Q(N/2) + O(1)$ I/Os

$\Rightarrow$ solves to $O\left(1 + N^2/B\right)$, optimal

Performance of Matrix Transposition [Chatterjee,Sen]

300 MHz UltraSPARC-II, 2 MB L2 cache, 16 KB L1 cache,
page size 8 KB, 64 TLB entries

Running time (seconds), $B = 32$

$\log_2 N$	Naive	I/O	CO
10	0.21	0.10	0.08
11	0.86	0.49	0.45
12	3.37	1.63	2.16
13	13.56	**6.38**	6.69

Running time (seconds), $B = 128$

$\log_2 N$	Naive	I/O	CO
10	0.14	0.12	0.09
11	0.87	0.42	0.47
12	3.36	1.46	2.03
13	13.46	**5.74**	6.86

$\Rightarrow$ Tuned cache-aware algorithm is faster then CO algorithm

$\Rightarrow$ CO algorithm is much faster than naive algorithm

Cache Simulator Results

$N = 2^{13}$, $B = 2^6$

Algorithm	Data refs	L1 misses	TLB misses
Naive	134 mln	38 mln	34 mln
I/O	403 mln	37 mln	0.3 mln
CO	134 mln	56 mln	2 mln

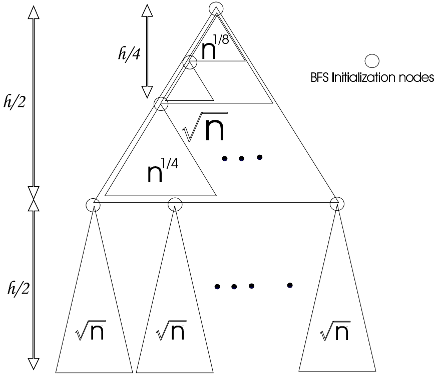
- Naive alg.: few data accesses but many non-local
- CO alg.: too deep recursion $\Rightarrow$ many L1 and TLB misses
- CO alg.: breaking recursion earlier gives better performance

Cache-Oblivious Searching

- Binary search: $\Theta(log_2 N)$ I/Os, suboptimal 
- B-tree (B-way search): $\Theta(log_B N)$ I/Os, but needs to know B 
- Cache-oblivious search with $\Theta(log_2 N)$ I/Os, possible?

CO Static Search Trees [Prokop99]

Recursive memory layout of a perfect binary tree(van Emde Boas layout):

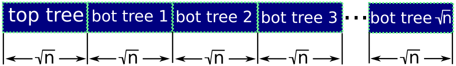


- Observation: if a subtree fits in a block its height is $\geq (\log B)/2$

$\Rightarrow$ a search crosses $O\left(\frac{\log n}{\log B}\right)$ subtrees

$\Rightarrow$ $O(\log_B n)$ I/Os

Memory layout:

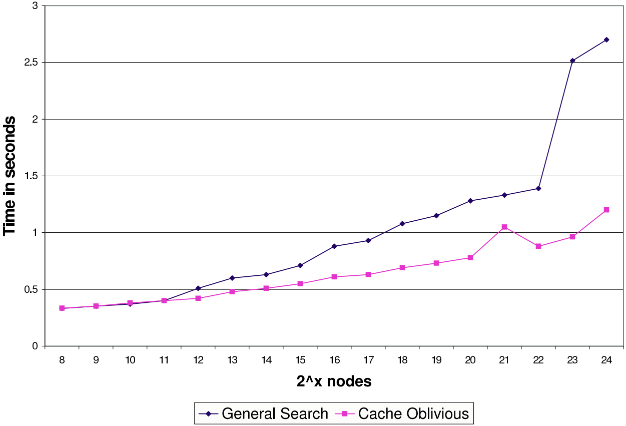


Experiments [Kumar2002]

Itanium processor, 2 GByte RAM, 48 byte elements, random input

General search $\equiv$ searching with pre-order layout

Cache-oblivious $\equiv$ searching with vEB layout



Cache-Oblivious Sorting

Simple recursive Mergesort: $Q(n) = 2Q(n/2) + \Theta(n/B)$

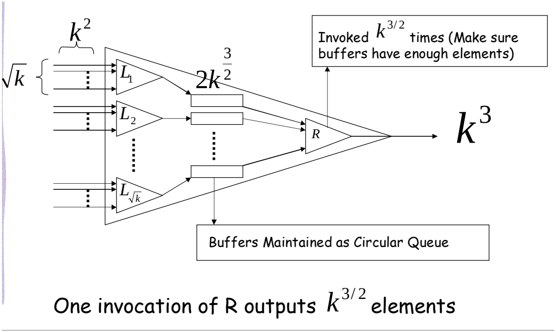
$\Rightarrow Q(n) = \Theta(\frac{N}{B}\log_2 \frac{N}{B})$ I/Os, suboptimal 

How to increase log base to M/B without knowning M and B?

Solution: a recursive merger (k-funnel) [Frigo et al. 1999]

K-funnel

- Input: k sorted sequences
- Outputs k^3 elements



- vEB layout:

R	B_1	L_1	B_2	L_2	B_3	L_3	$\ldots$	$B_{\sqrt{k}}$	$L_{\sqrt{k}}$

- Merging k^3 elements takes $\Theta(\frac{k^3}{B}\log_{M/B}(\frac{k^3}{B})+k)$ I/Os and $\Theta(\log_2 n)$ work

Lazy Funnelsort [BroFag2002]

1. Split input into $k = n^{1/3}$ contig. segments each of size $n/k = n^{2/3}$
2. Recursively sort each segment
3. Apply the k-**funnel** to merge the sorted sequences.

I/O-complexity: $Q(n) = n^{1/3}Q(n^{2/3}) + O\left((n/B)\log_{M/B}(n/B) + n^{1/3}\right)$
solves to $Q(n) = \frac{n}{B}\log_{M/B}(n/B)$

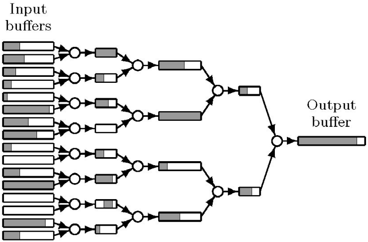
Practical?

A Practical Implementation [BroFagVin2004]

k-funnel structure:

- recursive implementation is faster than iterative (+ special allocator): Pentium 4 caches return instruction address
- navigation with pointers is faster than implicit layouts: too expensive CPU computation

Degree of Basic Mergers



- Tested mergers of degree $z = 2..9$: $z = 4$ is the optimum
  - small z: less instructions
  - large z: less levels, elements movements $1/\log(z)$, navigations

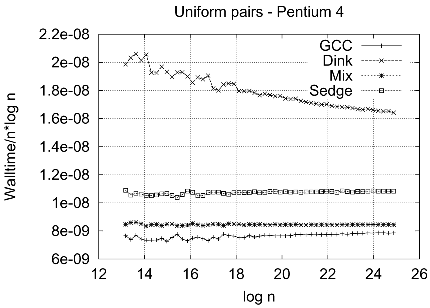
Other Optimizations

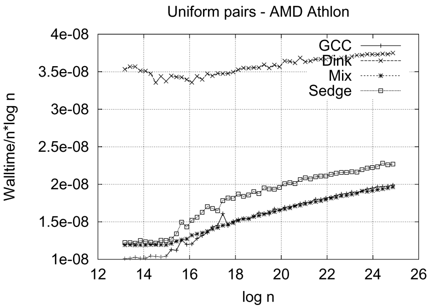
- Compute repeating merger configurations only once: 3-5 % speedup
- Base case: for < 100 elements use `std::sort`
- Tuning constants α,d for buffer lengths (αk^d)

  $\Rightarrow$ $\alpha = 16$, $d = 2.5$

Quicksort Implementations

GCC ≡ `std::sort` GCC C++ Version 3.2 implementation
Dink ≡ `std::sort` Dinkumware incl. in Intel C++ compiler 7.0, 3-way
Mix ≡ own implementtion of [BentleyMcIlroy93], 3-way partitioning
Sedge ≡ implementation by Sedgewick (book)

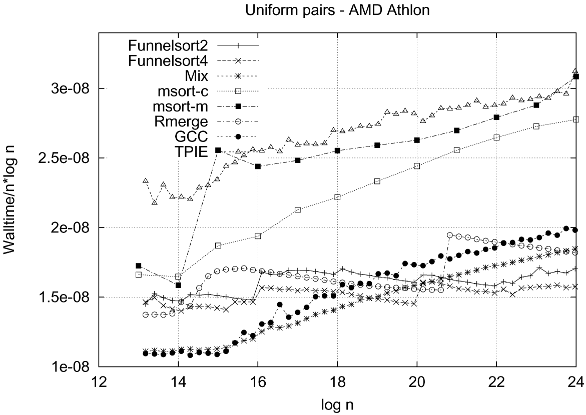




In-RAM Experiments

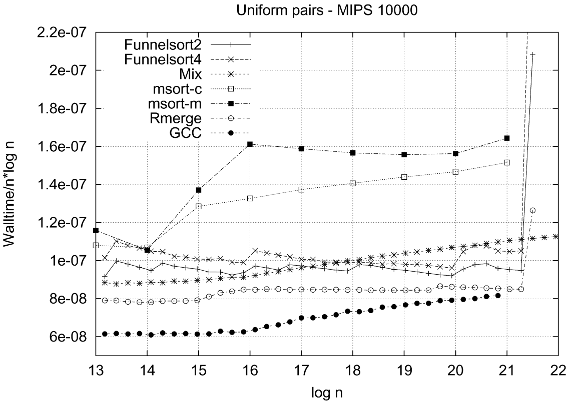
msort-* $\equiv$ cache-aware implementations from [Xioao et al. 2000]

Rmerge $\equiv$ cache-aware algorithm from [Arge et al. 2002]



Pentium III, Itanium 2: similar behavior

In-RAM Experiments on MIPS 10000



CPU cycles are costly

many registers

External Memory Experiments

Funnelsort run on inputs larger than M:

- use memory mapping (virtual memory):

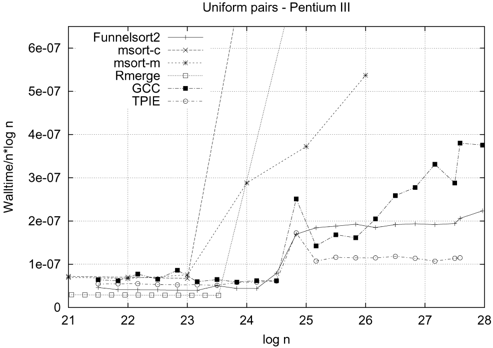
```
int * array;
mmap(&array,''filename'');
// algorithm begins

// reading memory:
var = array[i]; // file -> OS cache (RAM)->processor caches-> CPU
// if cache is full, flush data: CPU cache-> OS cache (RAM)->file

// writing memory:
array[j] = var2;
// checks caches, loads page from slower level if needed
// flush data if cache full

// algorithm finishes
munmap(array);
```

External Memory Experiments cont.



[Ajwani et al. 2007]:

n	Funnelsort	`stxxl::sort`
256×10^6	21 min	8 min
512×10^6	46 min	13 min
1024×10^6	96 min	25 min

$\Rightarrow$ **I/O-efficient/aware algorithms** tuned to external memory **perform better** (smaller constant factors, overlapping of I/O and computation)

Suffix Sorting

- Sort suffixes $T[i..n]$ of string $T[0..n]$.
- The result is Suffix Array: $SA[i]$ stores the position of ith smallest suffix
  - Powerful full-text search
  - Burrows-Wheeler text compression (UNIX `bzip2`)
  - Bioinformatics

Big interest in BIG inputs but no PRACTICAL I/O-efficient implementations existed !

Doubling

Lexicographic names

Choose integer name IDs such that:

$$T[i, i+2^k] \leq T[j, j+2^k] \text{ iff } \text{name}(T[i, i+2^k]) \leq \text{name}(T[j, j+2^k])$$

Doubling Algorithm

for $k := 1$ **to** $\lceil \log n \rceil$ **do**
    find lexicographic names for $T[i, i+2^k)$
    if the names are unique **then**
        return suffix array

How to generate names for the next iteration?

Idea: $T[i,i+2\cdot 2^k) \leq T[j,j+2\cdot 2^k)$
iff
$(\text{name}(T[i,i+2^k)),\text{name}(T[i+2^k,i+2\cdot 2^k))) \leq$
$(\text{name}(T[j,j+2^k)),\text{name}(T[j+2^k,j+2\cdot 2^k)))$

$\Rightarrow$

Name the pairs $(\text{name}(T[i,i+2^k)),\text{name}(T[i+2^k,i+2\cdot 2^k)))$
to get $\text{name}(T[i,i+2^{k+1}))$

Doubling Algorithm: Pseudocode

Function doubling(T)

$S:= \langle((T[i], T[i+1]), i) : i \in [0, n)\rangle$

for k := 1 **to** $\lceil \log n \rceil$ **do**

sort S

$P:=$ name(S)

invariant $\forall(c, i) \in P$:

c is a lexicographic name for $T[i, i+2^k)$

if the names in P are unique **then**

return $\langle i : (c, i) \in P\rangle$

sort P by $(i \textbf{ mod } 2^k, i \textbf{ div } 2^k)$

$S:= \langle((c, c'), i) : j \in [0, n),$

$(c, i) = P[j], (c', i+2^k) = P[j+1]\rangle$

Lexicographical Naming: Pseudocode

Function name$(S$: Sequence **of** Pair$)$

q:= r:= 0; (ℓ, ℓ'):= $(\$, \$)$

result:= $\langle\rangle$

foreach $((c, c'), i) \in S$ **do**

$q{+}{+}$

if $(c, c') \neq (\ell, \ell')$ **then** r:= q; (ℓ, ℓ'):= (c, c')

append (r, i) to result

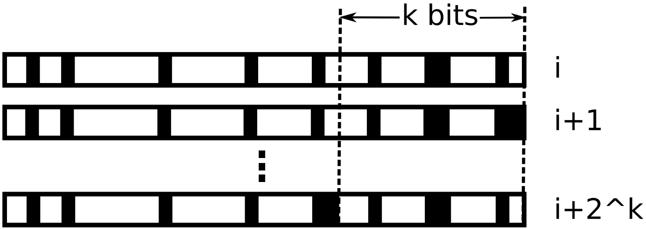
return result

Bit Shuffling

Problem: distance between name$(T[i, i+2^k))$ and name$(T[i+2^k, i+2\cdot 2^k))$ in P is 2^k

$\Rightarrow$ need two read pointers ($\times 2$ I/Os in the last iterations)

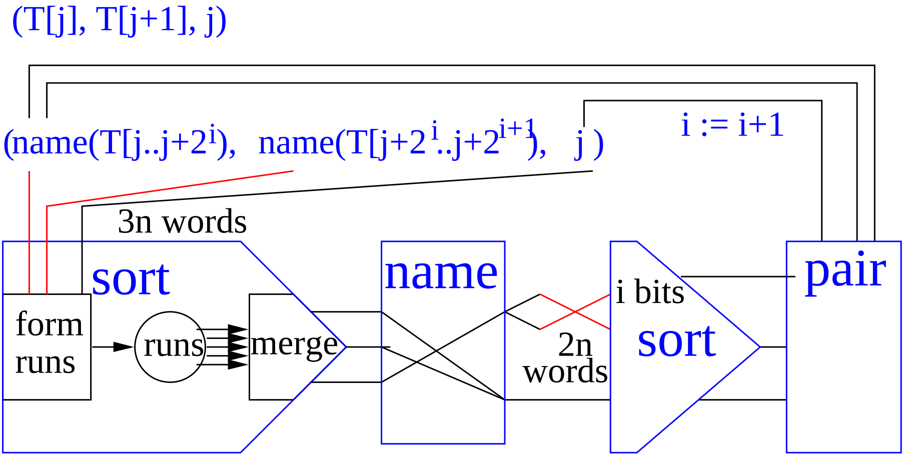
Solution: sort P by $(i \textbf{ mod } 2^k, i \textbf{ div } 2^k)$ instead of i



Doubling: Example

```
T = banana -> pair
<(ba,0), (an,1), (na,2), (an,3), (na,4), (a0,5)>
           -> sort by pairs
<(a0,5), (an,1), (an,3), (ba,0), (na,2), (na,4)>
           -> name
<( 1,5), ( 2,1), ( 2,3), ( 4,0), ( 5,2), ( 5,4)>
           -> shuffle by pos (mod 0, mod 1)
455 221    -> pair
<(45,0), (55,2), (50,4), (22,1), (21,3), (10,5)>
           -> sort by pairs
<(10,5), (21,3), (22,1), (45,0), (50,4), (55,2)>
           -> name
<( 1,5), ( 2,3), ( 3,1), ( 4,0), ( 5,4), ( 6,2)>
unique!    -> project -> 531042
```

Pipelined Doubling



total I/O complexity: $\mathrm{sort}(5n)\log \mathrm{maxlcp} + O(\mathrm{sort}(n))$

Discarding

Denote $c_i^k = \text{name}(T[i, i+2^k))$ (iteration k)

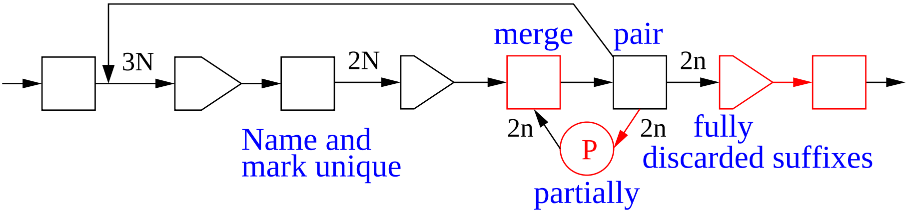
What if particular c_i^k is already unique?
$\Rightarrow$ Exclude suffix i from later iterations
$\Rightarrow$ Reduces I/O volume

The names are stable, i.e. if c_i^k is unique then $c_i^k = c_i^h$ for all $h > k$:

- Fully discard from S all tuples $((c, c'), i)$ where c is unique
  - Previous approaches [CF 97] scanned **all** discarded suffixes in **all** iterations
- Can not discard $((c, c'), i)$ if c' is unique but c is not
  - Partially discard (c, i) (keep in a separate EM array – **only scanned** in later iterations)

Pipelined Improved Discarding

- Scan all unique suffixes [CF 97]$\rightsquigarrow$
  Scan new unique suffixes
- Triples [Kärkkäinen 03]$\rightsquigarrow$ pairs



$$\mathrm{sort}(5N) + O(\mathrm{sort}(n)) \text{ I/Os where } N = \sum_i \log \mathrm{distPrefixSize}(T[i..n]))$$

a-Tupling

Sort by first a^i characters in iteration i

- large a: few iterations, but need to sorts long tuples
- small a: many iterations, sorting short tuples

Constant Factor in I/O Volume

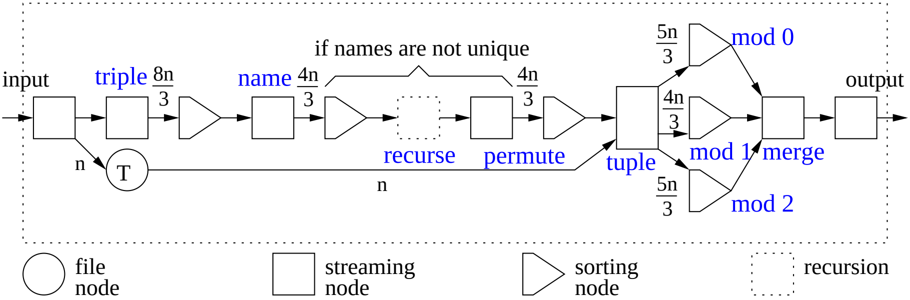
a	2	3	4	5	6	7
$(a+3)/\log a$	5.00	3.78	3.50	**3.45**	3.48	3.56

CPU computations for $a = 4$ are cheaper than for $a = 5$, I/O volume differs by **only** 1.5 %

Difference Cover 3 (DC3,Skew) Algorithm

1. sort $T[i..n]$ for $i \bmod 3 \in \{1,2\}$
   sort and name triples
   recurse
2. sort $T[i..n]$ for $i \bmod 3 \in \{0\}$
   sort pairs $(T[3i], \mathrm{name}(T[3i+1..n]))$
3. merge using difference cover property of $\{1,2\}$
   $T[3i..n] \le T[3j+1..n]$ iff
   $(T[3i\quad], \mathrm{name}(T[3i+1..n])) \le$
   $(T[3j+1], \mathrm{name}(T[3j+2..n]))$
   $T[3i..n] \le T[3j+2..n]$ iff
   $(T[3i\quad..3i+1], \mathrm{name}(T[3i+2..n])) \le$
   $(T[3j+2..3j+3], \mathrm{name}(T[3j+4..n]))$

Pipelined DC3



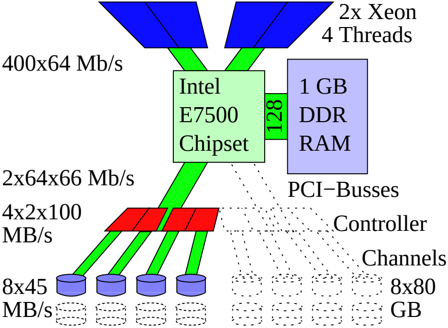
$\text{sort}(30n) + \text{scan}(6n)$ I/Os

Experimental Setup

Pipelining + STL-user layer from STXXL

Experiments on a faster machine (Opteron 1.8 GHz, SCSI Seagate 15,000 RPM disks) have shown **similar results**.

all computations took 30 days, 40 TBytes data moved



Inputs:

Genome: Human Genome (≈ 4GByte)

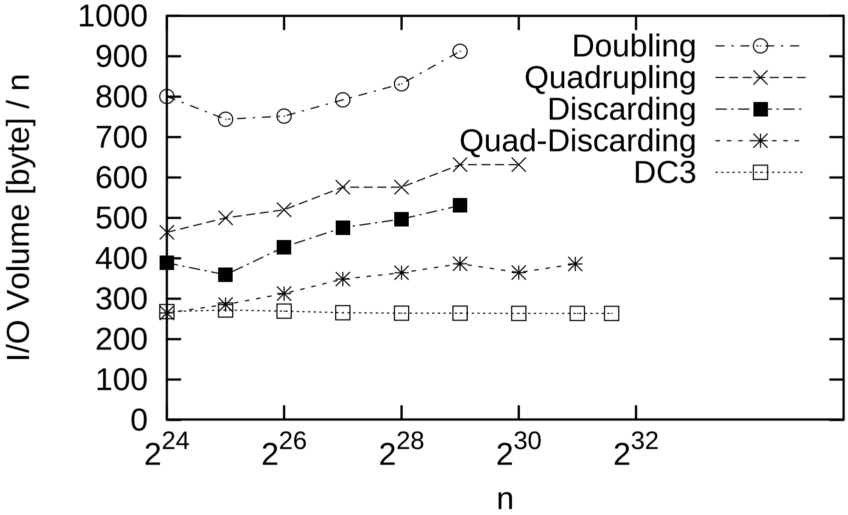
Gutenberg: ≈ 3GByte English text from Gutenberg project

HTML: ≈ 3GByte text from a crawl of `.gov`

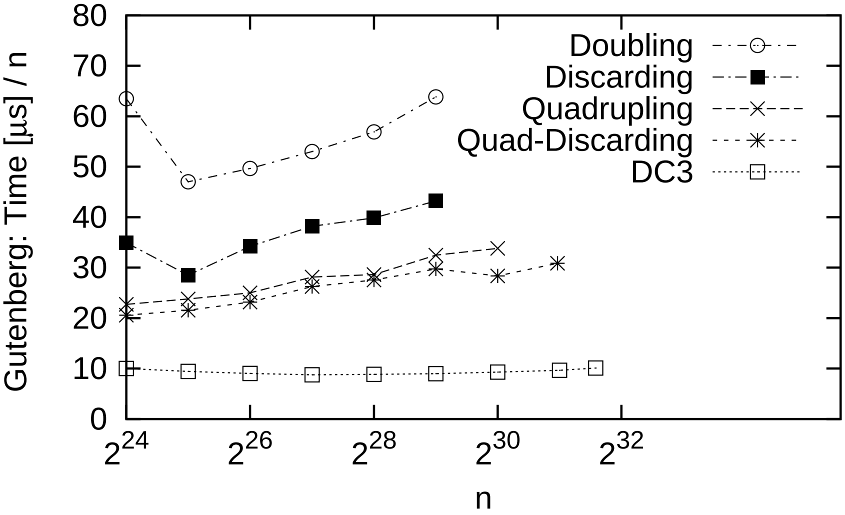
Source: ≈ 0.5GByte Linux sources

Random2: $T \circ T$ with $T := \mathrm{randChar}^{n/2}$

Gutenberg I/Os



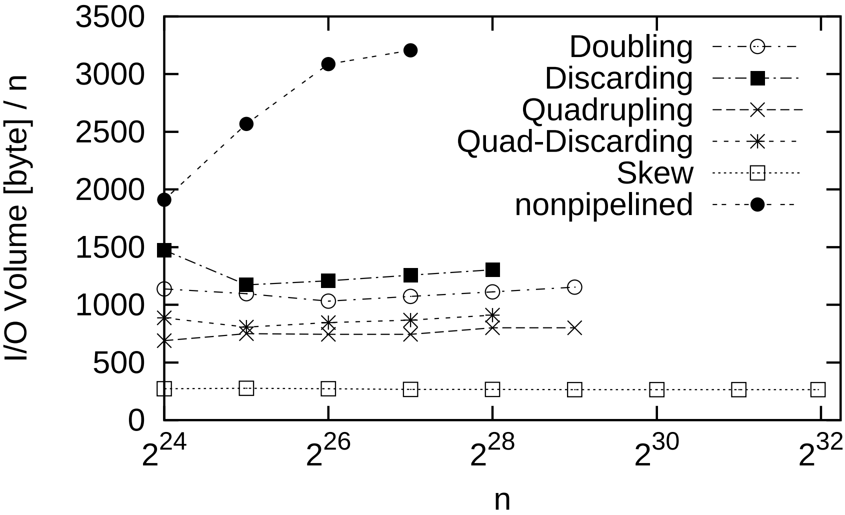
Gutenberg Time



Quadrupling is faster than doubling

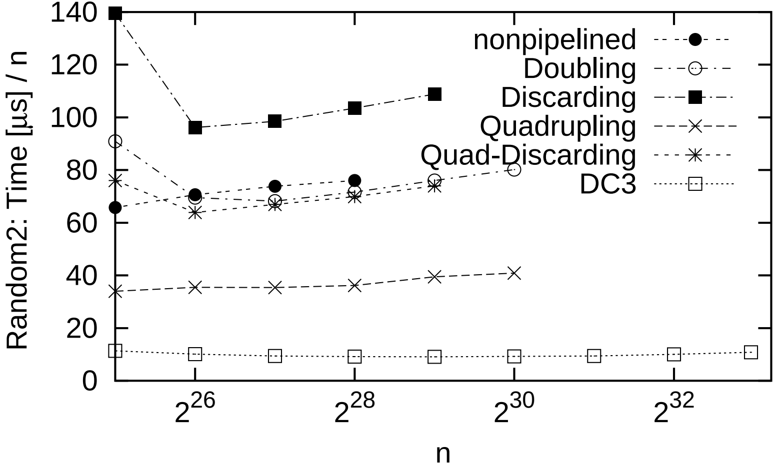
Discarding variants are faster (except special inputs)

Random2 I/Os



Non-pipelined doubling implementation has much larger I/O

Random2 Time



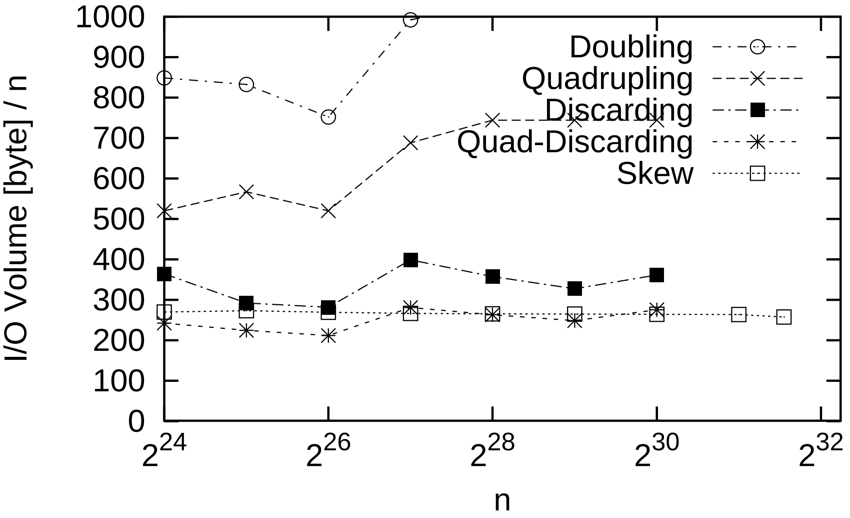
$D = 4 \Rightarrow$ fast I/O, less CPU work pays off:

non-pipelined doubling is close to pipelined doubling (for $D = 1$, speedup ≈ 2)

quadrupling **with discarding** loses quadrupling (complex CPU comput., difficult input)

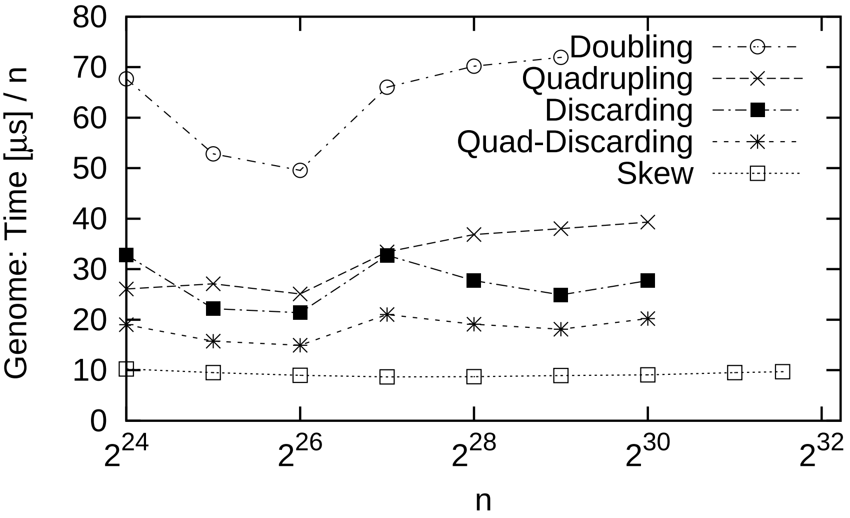
DC3 compares only pairs or triples vs. quadruples

Genome I/Os

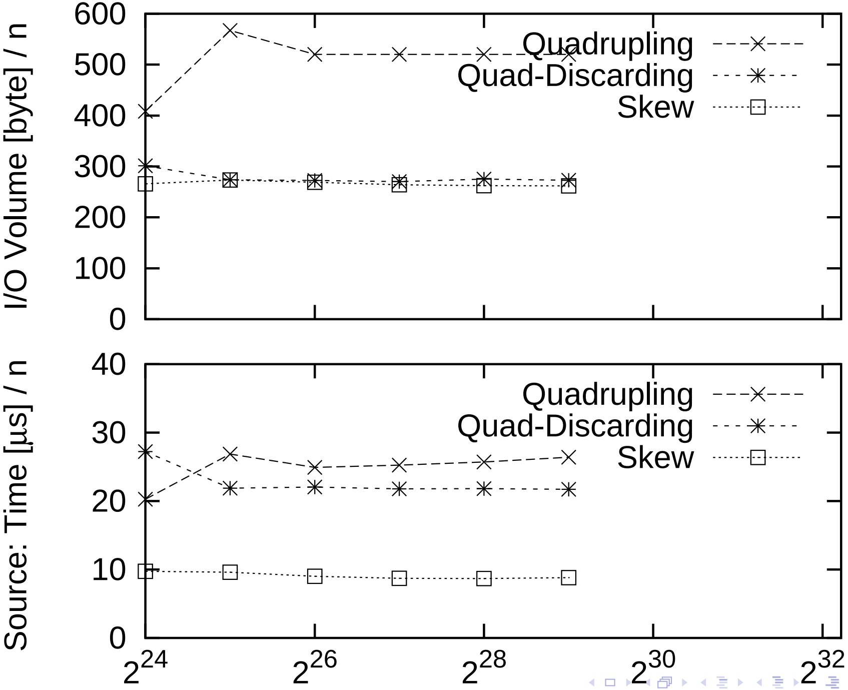


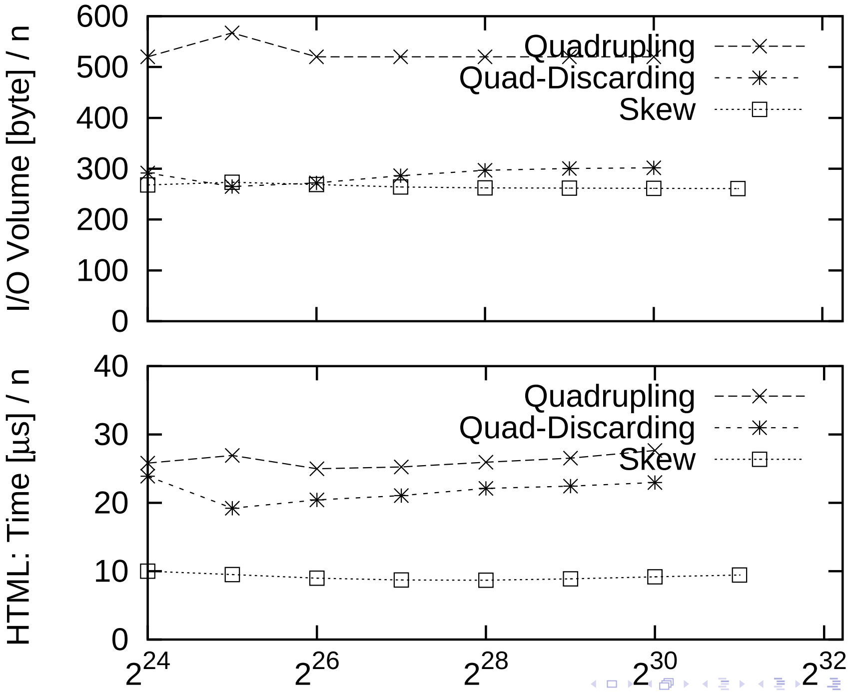
1000
900
800
700
600
500
400
300
200
100
0
I/O Volume [byte] / n
Doubling
Quadrupling
Discarding
Quad-Discarding
Skew
2^{24}
2^{26}
2^{28}
2^{30}
2^{32}
n

Genome Time



Genome: Time [µs] / n
80
70
60
50
40
30
20
10
0
Doubling
Quadrupling
Discarding
Quad-Discarding
Skew
2^{24}
2^{26}
2^{28}
2^{30}
2^{32}
n


I/O Volume [byte] / n
600
500
400
300
200
100
0
Quadrupling
Quad-Discarding
Skew
Source: Time [µs] / n
40
30
20
10
0
Quadrupling
Quad-Discarding
Skew
2^{24}
2^{26}
2^{28}
2^{30}
2^{32}


I/O Volume [byte] / n
600
500
400
300
200
100
0
Quadrupling
Quad-Discarding
Skew
HTML: Time [µs] / n
40
30
20
10
0
Quadrupling
Quad-Discarding
Skew
2^24
2^26
2^28
2^30
2^32

Comparison with Previous Implementations

- $5\times$ less I/Os than [CF 97]
- 7–$8\times$ less clock cycles than [CF 97] (including BGS algorithm)
- $2.4\times$ faster than internal compressed Genome [LSSSY 02]
- $1.2\times$ slower than internal Genome on 64 GByte super computer [Sadakane Shibuya 01]
- Faster than linear time internal LCP computation on MPII's SUN Starfire 15000

Other Hardware Configurations

DC3 with many disks

D	1	2	4	6	8
$t[\mu s/\text{byte}]$	13.96	9.88	8.81	8.65	8.52

$\Rightarrow$ CPU-bound $\Leftarrow$

A Faster 64-bit Opteron with SCSI disks

- Implementations are $1.7 - 2.4$ times faster
- Relative performance is the same

Conclusion

Results

- STXXL makes pipelining easy. Saves factor 2–3 in I/O volume.
- External DC3 is practical
- And better than pipelined 4-tupling with improved discarding

Future Work

- Tune pipelined sorters
- Go parallel
- Will discarding help for DC algorithms?

Terabytes over night?

DCX algorithm

choose suffixes starting at $I_X = \{i \mid i \mod X \in C_X\}$ (for DC3 $X = 3, C_3 = \{1, 2\}$)

for given X **minimize** C_X s.t. the order of the remaning suffixes can be reconstructed $\Rightarrow C_X = \{j \mid X - j - 1 \in C'_X\}$, where C'_X is minimum difference cover [Haanpää 2004]

X	C'_X
3	$\{0, 1\}$
7	$\{0, 1, 3\}$
13	$\{0, 1, 3, 9\}$
21	$\{0, 1, 6, 8, 18\}$
31	$\{0, 1, 3, 8, 12, 18\}$
39	$\{0, 1, 16, 20, 22, 27, 30\}$
57	$\{0, 1, 9, 11, 14, 35, 39, 51\}$
73	$\{0, 1, 3, 7, 15, 31, 36, 54, 63\}$
91	$\{0, 1, 7, 16, 27, 56, 60, 68, 70, 73\}$
95	$\{0, 1, 5, 8, 18, 20, 29, 31, 45, 61, 67\}$
133	$\{0, 1, 32, 42, 44, 48, 51, 59, 72, 77, 97, 111\}$

I/O-Volume Estimation of DCX

X	3	7	13	21	31	39	57
$\|C_X\|$	2	3	4	5	6	7	8
$\text{sort}[N]$	30	24.75	30.11	38.56	50.12	60.65	79.02
$\text{scan}[N]$	6	3.50	2.89	2.63	2.48	2.39	2.33
Total	66	**53**	63.11	79.75	102.72	123.75	160.37

DC7 has 20 % less I/O-volume than DC3

I/O-Volume Estimation of DCX with alphabet compression

Genome data (4-character alphabet): pack 16 characters in a 32-bit word

X	3	7	13	21	31	39	57
$\lvert C_X \rvert$	2	3	4	5	6	7	8
$\mathrm{sort}[N]$	24.50	18.17	15.46	15.23	15.14	16.57	17.43
$\mathrm{scan}[N]$	2.46	1.63	1.20	0.96	0.80	0.75	0.61
Total	**51.49**	37.99	32.13	31.41	31.09	33.89	35.49

more CPU work: practical ?

I/O-Efficient Spanning Trees

Simplify the MSF implementation [Schultes 2003]

- no "weight" component in tuples $\Rightarrow$ less I/Os
- base case simplified: no sorting needed for Kruskal's alg.
- delete node i:
  output the lightest edge $(i, w) \Rightarrow$ output (i, v) with
  $v = \min\{u : (i, u) \in E\}$

  $\Rightarrow$ postpone work to later iteration, faster reduction

EM Connected Components

Problem: for each node v find representative node $r(v)$ s.t. $r(v) = r(u)$ iff u and v are in the same component ($\exists$ path between u and v)

Adapt the MSF implementation using ideas from [Sibeyn and Meyer]

Preliminaries:

- "question" (v, u) is a preliminary assignment $u = r(v)$
- "answer" (v, u) is the ultimate asignment $u = r(v)$
- assignment of nodes to buckets $b : V \to \{0..k-1\}$

EM Connected Components: Pseudocode 1

During the processing of bucket i

if list of v is empty **then** $r(v) := v$ **else** $r(v) :=$ smallest entry in the list of v;

After the processing of bucket i

for $v := u_{i-1} + 1$ **to** u_i **do**
    if $r(v) \leq u_{i-1}$ **then**
        add $(v, r(v))$ to Questions[$b(r(v))$];
    else
        $r(v) := r(r(v))$;
        if $r(v) \leq u_{i-1}$ **then**
            add $(v, r(v))$ to Questions[$b(r(v))$];
        else
            add $(v, r(v))$ to Answers[$b(v)$];

EM Connected Components: Post-Processing

Post-Processing (An additional pass)

for $i := 1$ **to** b **do**
  read Answers[i];
  foreach $(v, r(v)) \in$ Questions[i] **do**
    $r(v) := r(r(v))$;
    add $(v, r(v))$ to Answers[b(v)];
  write Answers[i] to result;

Measurements: Speedup over the MSF implementation

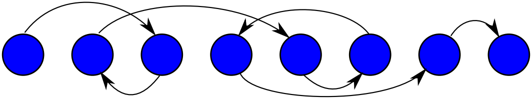
type	$n/10^6$	$m/10^6$	SF	CC	SF&CC
grid	80	160	7.1	5.8	5.8
grid	1280	2560	1.8	1.8	1.5
random	80	160	2.1	2.0	2.0
random	1280	2560	2.1	2.3	1.9
random	40	320	2.5	2.4	2.4
random	320	2560	2.1	2.5	2.0
geometric	80	149	2.8	2.4	2.4
geometric	640	1190	1.7	1.6	1.4
geometric	40	270	3.6	3.4	3.5
geometric	160	1080	3.3	3.2	3.2

- SF&CC is faster than MSF (factor ≥ 1.4)
- CC (without SF) does not carry original node ids
- SF is faster than CC: no third pass is needed, simple CPU work

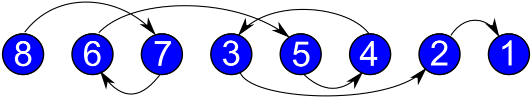
List Ranking

A fundamental graph problem: compute the **distance** to the list **tail**/head for each node in a list

Input (succ links):

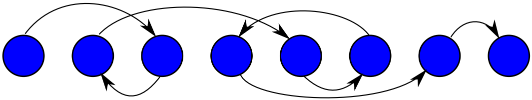


Output (node_id,dist):

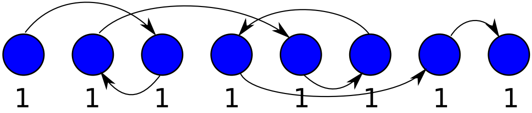


Internal memory algorithm (just follow links): $\Omega(n)$ I/Os

External Memory List Ranking

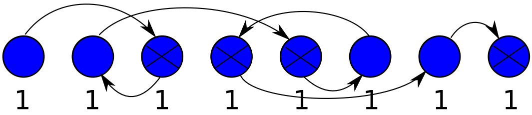


External Memory List Ranking



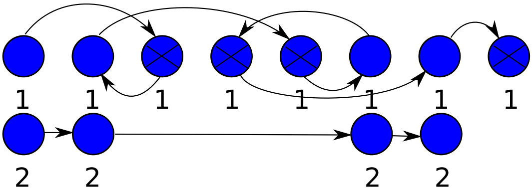
$dist[i] := 1,\ 1 \leq i \leq n$

External Memory List Ranking



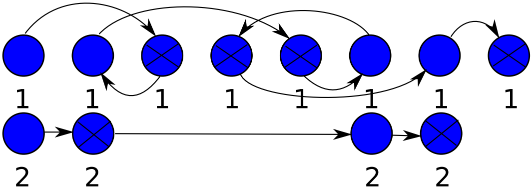
find a **Maximal Indepepen-dent Set** S $\Rightarrow$ $O(\mathrm{sort}(n))$ I/Os

External Memory List Ranking



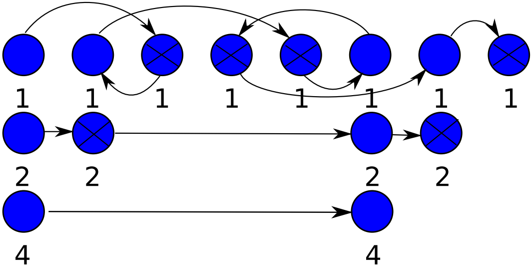
delete S and update $dist$: $dist[pred[i]] += dist[i]$, $i \in S$
$\Rightarrow O(\text{sort}(n))$ I/Os

External Memory List Ranking



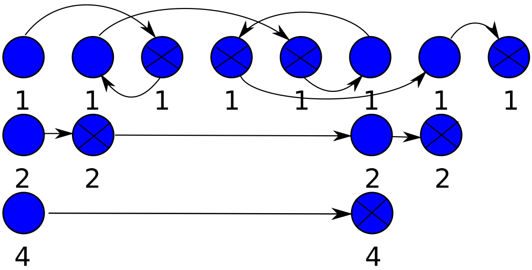
Find a MIS S

External Memory List Ranking



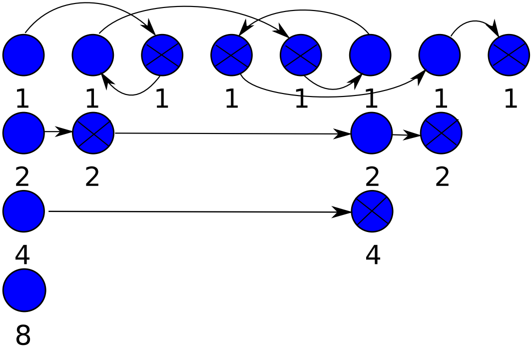
delete S and update *dist*:
$dist[pred[i]] += dist[i]$, $i \in S$

External Memory List Ranking



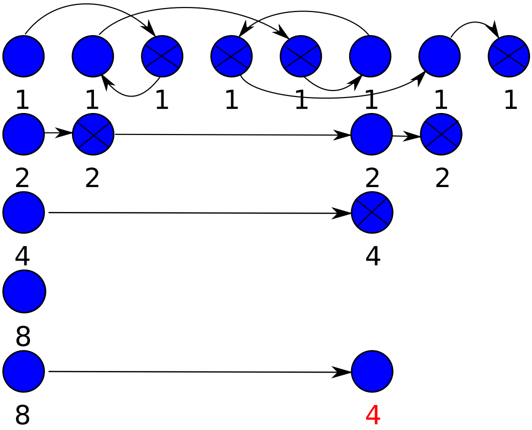
Find a MIS S

External Memory List Ranking



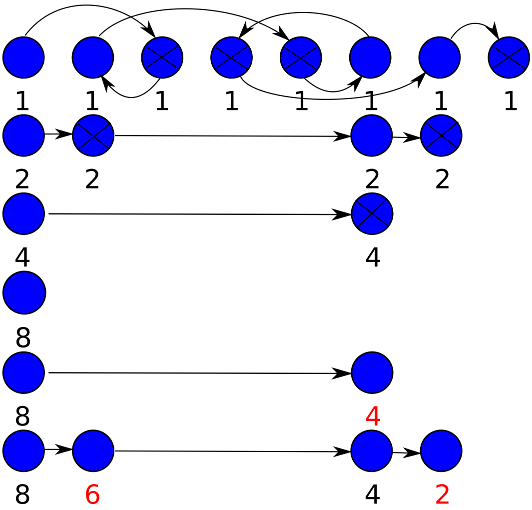
delete S and update *dist*:
$dist[pred[i]] += dist[i]$, $i \in S$

External Memory List Ranking



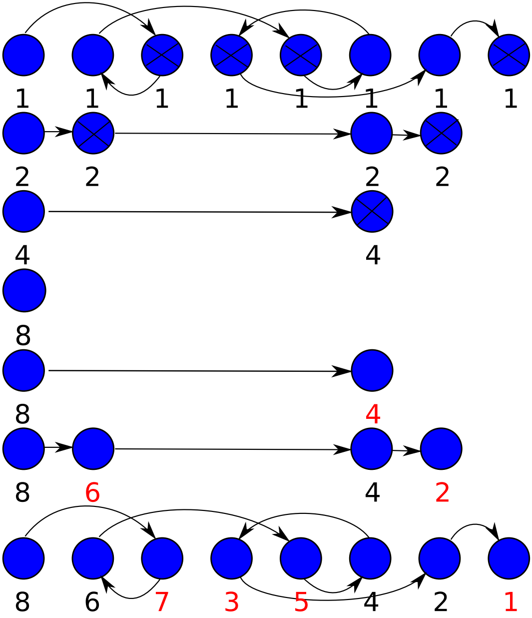
restore *S* and update *dist*:
$dist[i] += dist[succ[i]];, i \in S$

External Memory List Ranking



restore S and update *dist*:
$dist[i] += dist[succ[i]];$, $i \in S$

External Memory List Ranking



restore S and update *dist*:
$dist[i] += dist[succ[i]]$;, $i \in S$

EM List Ranking: Analysis

- Recursion step: $O(\mathrm{sort}(n))$ I/Os
- MIS on a list: $|S| \geq n/3$

$$\Rightarrow Q(n) \leq O(\mathrm{sort}(n)) + Q(2n/3) = O(\mathrm{sort}(n)) \text{ I/Os}$$

Not really practical, large I/O volume 

A More Practical Algorithm [Sibeyn2004]

The idea

- Similar to Connected Components Alg. [Sibeyn Meyer]
- Each node v keeps a (adjacency) list of entries (u, l):
  distance between v and u is l (can be negative)

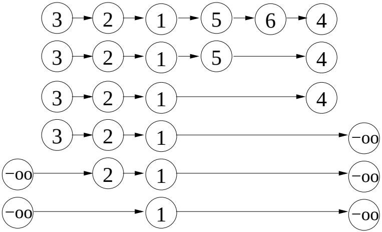
Fast List Ranking: Pseudocode

foreach edge $(u,v) \in L$ // Step 1
  if $u < v$ **then** add $(u,-1)$ to the list of v
  else add $(v,1)$ to the list of u
for $u := n-1$ **downto** 1 **do** // Step 2
  if u has list entries (v,l_v) and (w,l_w), $v < w < u$ **then**
    add $(v,l_v - l_w)$ to the list of w
  else // u has a single entry (w,l_w), $w < u$
    add $(-\infty,-l_w)$ to the list of w
  $ref_u := w$
  $\delta_u := l_w$
// node 0 has list entries $(-\infty,l_{head})$, $l_{head} < 0$ and/or $(-\infty,l_{tail})$, $l_{tail} > 0$
$d(0) := l_{last}$ or 0 if node 0 is the tail // distance from the last node
for $u := 1$ **to** $n-1$ **do** // Step 3
  $d(u) := d(ref_u) + \delta_u$

Fast List Ranking: Example (Step 2)

(the list nodes are ordered for the simplicity)

1	2	3	4	5	6
	(1,1)	(2,1)		(1,-1)	(5,-1) (4,1)
	(1,1)	(2,1)		(1,-1) (4,2)	
	(1,1)	(2,1)	(1,-3)		
$(-\infty,3)$	(1,1)	(2,1)			
$(-\infty,3)$	(1,1) $(-\infty,-1)$				
$(-\infty,3)$ $(-\infty,-2)$					



Fast List Ranking: Analysis

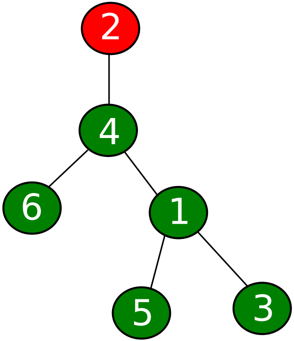
- Message sending and receiving: an I/O-efficient priority queue
- Each step has n iterations
- Each iteration step performs $O(1)$ PQ operations

$\Rightarrow$ Total: $O(\mathrm{sort}(n))$ I/Os

Possible Implementation

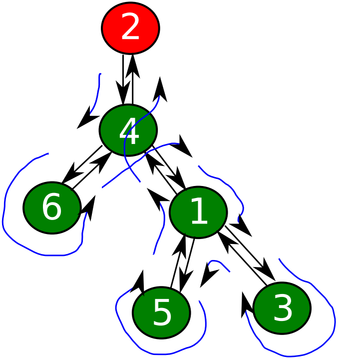
- Instead of PQ can use buckets (linear CPU work)
- Estimation from [Sibeyn2004]: $\times 4$ faster than the MIS-based algorithm

Euler Tour



Input:

$(2,4),(4,1),(4,6),(3,1),(5,1)$



Output:

$[(2,4),(4,6)],[(6,4),(4,1)],[(4,6),(6,4)],$
$[(4,1),(1,3)],[(3,1),(1,5)],[(5,1),(1,4)],$
$[(1,3),(3,1)],[(1,4),(4,2)],[(1,5),(5,1)]$

no specific order!!

EM Euler Tour Algorithm

- Let $(v, w_1), \ldots, (v, w_k)$ are incident edges of v
- $succ((w_i, v)) = (v, w_{i+1})$ for $1 \leq i < k$ and $succ((w_k)) = (v, w_1)$

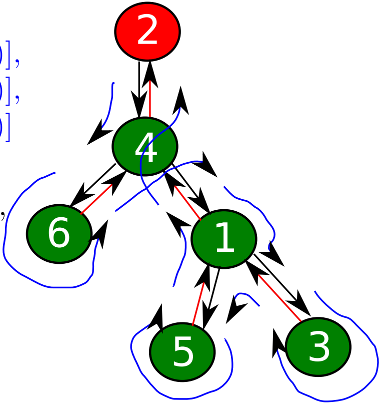
Algorithm

1. Scan E to replace (v, w) with (v, w) and (w, v)
2. Sort the result by target node ids (groups incoming edges together)
3. Scan the result to compute $[(v, w), succ((v, w))]$ pairs

$\Rightarrow O(\mathrm{sort}(n))$ I/Os

Euler Tour Technique

Many applications: e.g. tree rooting (direct each edge from parent to the child)



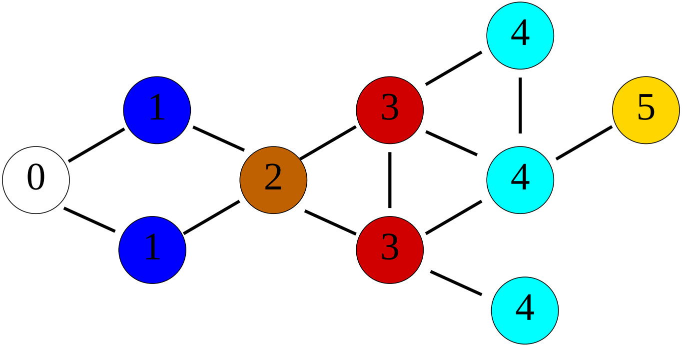
1. Compute Euler Tour
   $[(2,4),(4,6)],[(6,4),(4,1)],[(4,6),(6,4)],$
   $[(4,1),(1,3)],[(3,1),(1,5)],[(5,1),(1,4)],$
   $[(1,3),(3,1)],[(1,4),(4,2)],[(1,5),(5,1)]$
2. Run list ranking
   $[(2,4),10],[(4,6),9],[(6,4),8],[(4,1),7],$
   $[(1,3),6],[(3,1),5],[(1,5),4],[(5,1),3],$
   $[(1,4),2],[(4,2),1]$
3. Sort edges $[(u,v),d]$ by
   $(\min(u,v),\max(u,v))$
   and for opposite edges (u,v) and (v,u)
   take ones with smaller rank
   $[(1,3),6],[(3,1),5],[(1,4),2],[(4,1),7],$
   $[(1,5),4],[(5,1),3],[(2,4),10],[(4,2),1],$
   $[(4,6),9],[(6,4),8]$

$\Rightarrow O(\text{sort}(n))$ I/Os

Other Tree Algorithms using Euler Tour/List Ranking

- Subtree size
- Distance to root
- Preorder numberung
- Postorder numbering
- . . .

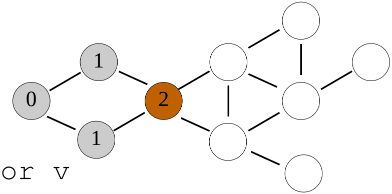
Breadth First Search



- Applications: state exploration, shortest paths, crawling WWW, ...

BFS: Internal Memory Algorithm

```
Q: FIFO queue of nodes
Q.push(s)
while Q.notEmpty()
  u := Q.pop();
  visit u
  foreach unmarked neighbor v
    mark v
    Q.push(v)
```



BFS: Internal Memory Algorithm

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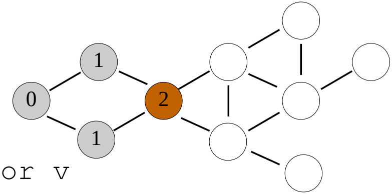
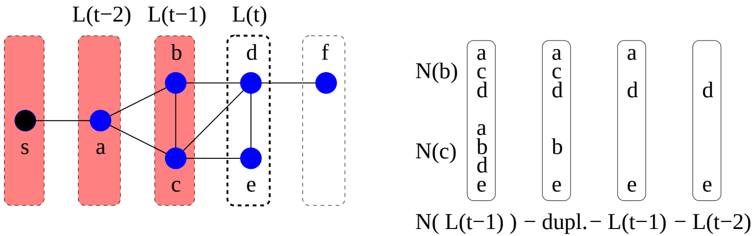


- Marking nodes: $\Theta(m)$ I/Os
- Finding neighbors (adj. lists): $\Theta(n)$ I/Os

Algorithm of Munagala and Ranade

Creating BFS level t (node set $L(t)$):
all reached neighbors of nodes in $L(t-1)$ belong to $L(t-2)$ or $L(t-1)$.

1. $N(L(t-1))$ = all neighbours of $L(t-1)$ — $\mathcal{O}\left(|L(t-1)| + \frac{|N(L(t-1))|}{D \cdot B}\right)$ I/Os.
2. eliminate duplicates in $N(L(t-1))$ by sorting — $\mathcal{O}(\mathrm{sort}(|N(L(t-1))|))$ I/Os.
3. eliminate nodes already in $L(t-1)$ by scanning — $\mathcal{O}(\mathrm{scan}(|L(t-1)|))$ I/Os.
4. eliminate nodes already in $L(t-2)$ by scanning — $\mathcal{O}(\mathrm{scan}(|L(t-2)|))$ I/Os.



$\sum_i |N(L(i))| \leq 2 \cdot m$ and $\sum_i |L(i)| \leq n \Rightarrow \mathcal{O}(n + \mathrm{sort}(n+m))$ I/Os in total.

Algorithm of Mehlhorn and Meyer

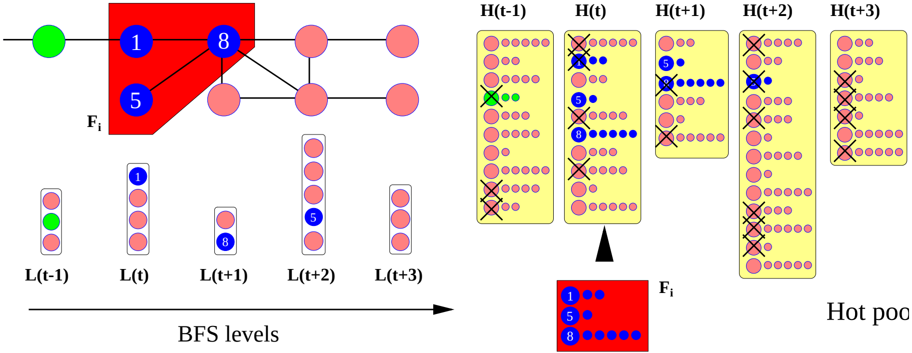
Preprocessing: $\mathcal{O}(\mathrm{sort}(n+m))$ I/Os

- partition nodes into $\mathcal{O}(n/\mu)$ subsets (clusters) s.t. any two nodes in same cluster have distance at most μ in G.
- store adjacency lists of nodes in the same cluster consecutively

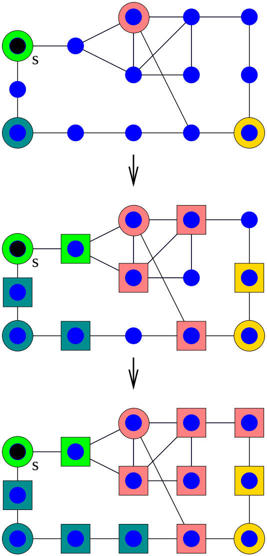
BFS Phase: Refined Algorithm of Munagala-Ranade

- extract neighbors of $L(t)$ by scanning sorted external data structure $\mathcal{H}$ (hot pool) – prevents the $O(n)$ accesses.
- if first node in a cluster is reached, add all adjacency lists of the cluster to $\mathcal{H}$.
- each adjacency list stays in $\mathcal{H}$ for at most μ **iterations.**
- $\mathcal{O}\left(n/\mu + \mu \cdot \mathrm{scan}(n+m) + \mathrm{sort}(n+m)\right)$ I/Os.
- **Balancing:** $\mathcal{O}\left(\sqrt{nm/B} + \mathrm{sort}(n+m)\right)$ **I/Os**.

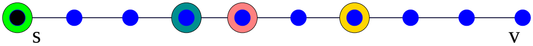
BFS Phase: Example



Randomized Clustering



- choose n/μ random master nodes.
- grow subgraphs S_i around master nodes in parallel: Label unvisited neighbor nodes & discard them from the representation of G.
- any node is labeled after $\mathcal{O}(\mu)$ phases on average.



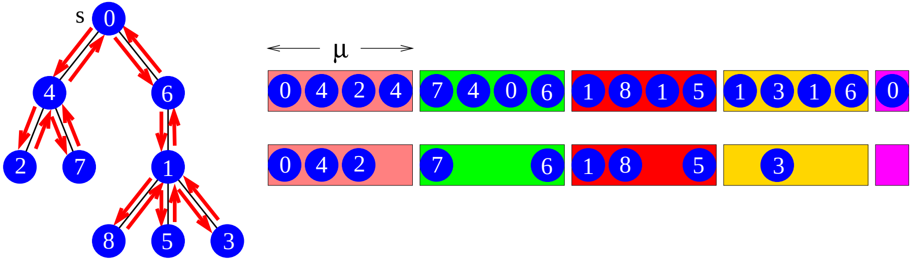
- I/Os per phase (F = fringe = active nodes):
  $\mathcal{O}(\mathrm{sort}(|F|+|N(F)|)+\mathrm{scan}(|G_{\text{unvisited}}|))$

$\Rightarrow$ $\mathcal{O}(\mu \cdot \mathrm{scan}(n+m)+\mathrm{sort}(n+m))$
expected I/Os for partitioning.

$\Rightarrow$ $\forall u,v \in S_i \ : \ \mathrm{dist}(u,v)$ in $G = \mathcal{O}(\mu \cdot \log n)$ whp.

Deterministic Clustering

1. Build a spanning tree: $\mathcal{O}(\text{sort}(n+m))$ I/Os (randomized).
2. Obtain Euler-tour (length $2n$) and do list ranking: $\mathcal{O}(\text{sort}(n))$ I/Os.
3. Chop Euler-tour into $2n/\mu$ pieces.
4. Eliminate duplicates: $\mathcal{O}(\text{sort}(n))$ I/Os.

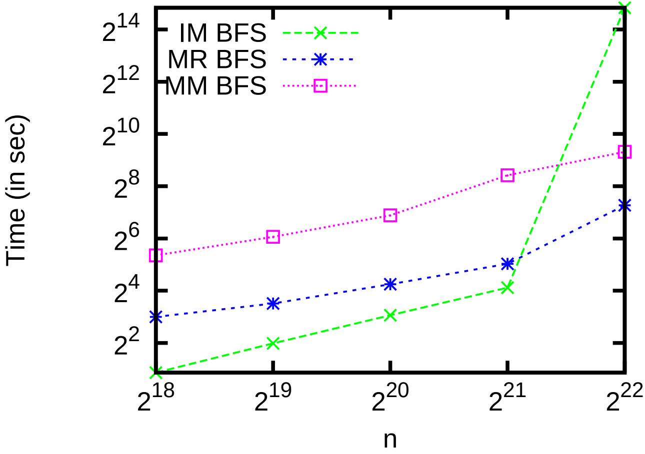


$\Rightarrow \mathcal{O}(\text{sort}(n+m))$ I/Os for partitioning.

Experiments

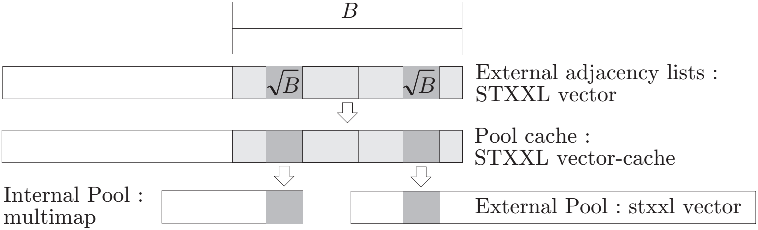
2.0 GHz Opteron, 1 GByte RAM, 250 GByte PATA Seagate disk (65 MByte/s, 9 ms seek time)

IM BFS vs. pipelined MR BFS and MM BFS (STXXL)



Tuning MM BFS [Ajwani et al. 2006]

- Choose fast EM list ranking, CC, MSF subroutines (earlier).
- Tune: # clusters, block sizes etc.
- Efficient implementation of internal-memory pools and cluster prefetching.



- "Randomize" the shape of underlying spanning trees (det. variant).
  $\rightsquigarrow$ Smaller cluster diameters

A few numbers

Total running times in hours:

Graph class	n	MunRan	MehMey_Rand	MehMey_Det
Random, $m = 4n$	2^{28}	1.4 **h**	$7\times$	$6\times$
Webgraph $m \simeq 8n$	2^{27}	2.6 **h**	$3.5\times$	$2\times$
Random Grid $(2^{14} \times 2^{14})$	2^{28}	$2.5\times$	$1.25\times$	21 **h**
Random Grid $(2^{21} \times 2^{7})$	2^{28}	$> 100\times$	$> 10\times$	4.0 **h**
Random Grid $(2^{27} \times 2)$	2^{28}	$> 500\times$	$> 25\times$	3.8 **h**
Random Line	2^{28}	$> 1000\times$	$> 25\times$	3.7 **h**
Simple Line	2^{28}	0.4 **h**	$7\times$	$7\times$
Max.		$\sim 1/2$ year	$\sim$ 1 week	$\sim$ 1 day

Other Experiments

Parallel disks ($D = 4$)

- Speedup is about two
- Become more CPU bound: may benefit from parallel processing in STXXL sorting

Cache Oblivious Implementation[Christiani]

- Uses CO sorting, CO list ranking, CO MST
- Factor 14-20 slower than EM implementation

EM BFS: Conclusion

- IM-BFS clearly worst on most external instances.
- **[MunRan99] better** than [MehMey02] **on well-behaved instances** (typ. 1 hour vs. 5 hours).
- **[MehMey02_Det] much better** than [MunRan99] **on difficult instances** (typ. 4 hours vs. 1/2 year).
- **[MehMey02_Det]** proved to be the **most robust choice**.
- Undirected EM-BFS becomes feasible.

The big challenge for the future:

Directed EM-BFS.