## CS 240 - Data Structures and Data Management

## Module 11: External Memory

T. Biedl E. Kondratovsky M. Petrick O. Veksler Based on lecture notes by many previous cs240 instructors

David R. Cheriton School of Computer Science, University of Waterloo

Winter 2022

#### Outline

- External Memory
  - Motivation
  - Stream-based algorithms
  - External sorting
  - External Dictionaries
  - 2-4 Trees
  - *a-b*-Trees
  - B-Trees

#### Outline

- External Memory
  - Motivation
  - Stream-based algorithms
  - External sorting
  - External Dictionaries
  - 2-4 Trees
  - a-b-Trees
  - B-Trees

## Different levels of memory

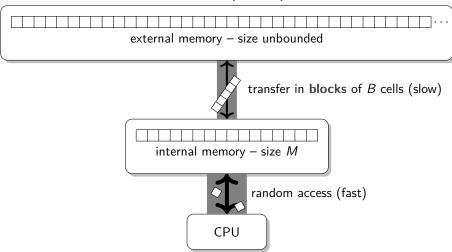
#### Current architectures:

- registers (very fast, very small)
- cache L1, L2 (still fast, less small)
- main memory
- disk or cloud (slow, very large)

General question: how to adapt our algorithms to take the memory hierarchy into account, avoiding transfers as much as possible?

**Observation**: Accessing a single location in *external memory* (e.g. hard disk) automatically loads a whole **block** (or "page").

# The External-Memory Model (EMM)



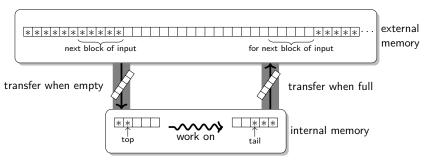
New objective: revisit all algorithms/data structures with the objective of minimizing block transfers ("probes", "disk transfers", "page loads")

#### Outline

- External Memory
  - Motivation
  - Stream-based algorithms
  - External sorting
  - External Dictionaries
  - 2-4 Trees
  - a-b-Trees
  - B-Trees

# Streams and external memory

If input and output are handled via streams, then we automatically use  $\Theta(\frac{n}{B})$  block transfers.



So can do the following with  $\Theta(\frac{n}{B})$  block transfers:

- Pattern matching: Karp-Rabin, Knuth-Morris-Pratt, Boyer-Moore (This assumes that pattern P fits into internal memory.)
- Text compression: Huffman, run-length encoding, Lempel-Ziv-Welch

#### Outline

- 11 External Memory
  - Motivation
  - Stream-based algorithms
  - External sorting
  - External Dictionaries
  - 2-4 Trees
  - a-b-Trees
  - B-Trees

# Sorting in external memory

Recall: The sorting problem:

Given an array A of n numbers, put them into sorted order.

Now assume n is huge and A is stored in blocks in external memory.

- Heapsort was optimal in time and space in RAM model
- But: Heapsort accesses A at indices that are far apart
  - → typically one block transfer per array access
  - $\rightsquigarrow$  typically  $\Theta(n \log n)$  block transfers.

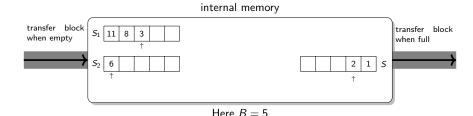
Can we do better?

- Mergesort adapts well to external memory. Recall algorithm:
  - Split input in half
  - lacktriangle Sort each half recursively o two sorted parts
  - Merge sorted parts.

Key idea: Merge can be done with streams.

# Merge

```
\begin{aligned} &\textit{Merge}(S_1, S_2, S) \\ &S_1, S_2 \text{: input streams have items in sorted order, } S \text{: output stream} \\ &1. & \textbf{while } S_1 \text{ or } S_2 \text{ is not empty } \textbf{do} \\ &2. & \textbf{if } (S_1 \text{ is empty}) \ S.\textit{append}(S_2.\textit{pop}()) \\ &3. & \textbf{else if } (S_2 \text{ is empty}) \ S.\textit{append}(S_1.\textit{pop}()) \\ &4. & \textbf{else if } (S_1.top() < S_2.top()) \ S.\textit{append}(S_1.\textit{pop}()) \\ &5. & \textbf{else } S.\textit{append}(S_2.\textit{pop}()) \end{aligned}
```



# Mergesort in external memory

- Merge uses streams  $S_1, S_2, S$ .
  - $\Rightarrow$  Each block in the stream only transferred once.
- So Merge takes  $\Theta(\frac{n}{B})$  block-transfers.
- Recall: Mergesort uses [log<sub>2</sub> n] rounds of merging.
- $\Rightarrow$  Mergesort uses  $O(\frac{n}{B} \cdot \log_2 n)$  block-transfers.

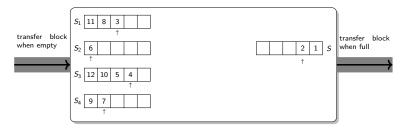
Not bad, but we can do better.

## Towards *d*-way Mergesort

**Observe:** We had space left in internal memory during *merge*.



- We use only three blocks, but typically  $M \gg 3B$ .
- Idea: We could merge d parts at once.
- Here  $d \approx \frac{M}{B} 1$  so that d+1 blocks fit into internal memory.

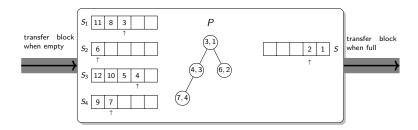


#### d-way merge

```
d-way-merge(S_1, \ldots, S_d, S)
```

 $S_1, \ldots, S_d$ : input streams have items in sorted order, S: output stream

- 1.  $P \leftarrow \text{empty } min\text{-}oriented \text{ priority queue}$
- 2. **for**  $i \leftarrow 1$  to d **do**  $P.insert((S_i.top(),i))$  // each item in P keeps track of its input-steam
- 3. **while** *P* is not empty **do**
- 4.  $(x, i) \leftarrow P.deleteMin()$
- 5.  $S.append(S_i.pop())$
- 6. **if**  $S_i$  is not empty **do**  $P.insert((S_i.top(),i))$



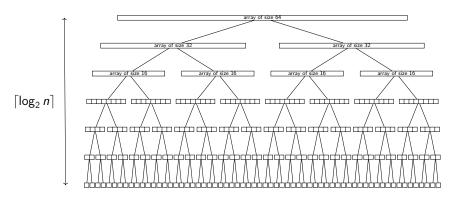
### d-way merge

- We use a min-oriented priority queue P to find the next item to add to the output.
  - ► This is irrelevant for the number of block transfers.
  - ► But there is no space-overhead needed for a priority queue. (Recall: heaps are typically implemented as arrays.)
  - ▶ And with this the run-time (in RAM-model) is  $O(n \log d)$ .
- The items in P store not only the next key but also the index of the stream that contained the item.
  - ▶ With this, can efficiently find the stream to reload from.
- We assume d is such that d+1 blocks and P fit into main memory.
- The number of block transfers then is again  $O(\frac{n}{B})$ .

How does *d-way merge* help to improve external sorting?

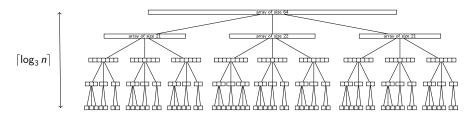
## Towards *d*-way Mergesort

Recall: Mergesort uses  $\lceil \log_2 n \rceil$  rounds of splitting-and-merging.



## Towards *d*-way Mergesort

**Observe:** If we split and merge d-ways, there are fewer rounds.



- Number of rounds is now  $\lceil \log_d n \rceil$
- We choose d such that each round uses  $\Theta(\frac{n}{B})$  block transfers. (Then the number of block transfers is  $\Theta(\log_d n \cdot \frac{n}{B})$ .)
- Two further improvements:
  - ► Proceed bottom-up (while-loops) rather than top-down (recursions).
  - $\blacktriangleright$  Save more rounds by starting immediately with runs of length M.

# d-way mergesort

External (B = 2):

39 5 28 22 10 33 29 37 8 30 54 40 31 52 21 45 35 11 42 53 13 12 49 36 4 14 27 9 44 3 32 15 43 2 17 6 46 23 20 1 24 7 18 47 26 16 48 50

Internal $(M = 8)$ :							

- ① Create  $\frac{n}{M}$  sorted runs of length M.  $\Theta(\frac{n}{B})$  block transfers
- ② Merge the first  $d \approx \frac{M}{B} 1$  sorted runs using d-Way-Merge
- ③ Keep merging the next runs to reduce # runs by factor of d  $\rightsquigarrow$  one round of merging.  $\Theta(\frac{n}{B})$  block transfers
- 4 Keep doing rounds until only one run is left

## d-way mergesort

- We have  $\log_d(\frac{n}{M})$  rounds of merging:
  - $ightharpoonup \frac{n}{M}$  runs after initialization
  - $ightharpoonup \frac{m}{M}/d$  runs after one round.
  - $\frac{n}{M}/d^k$  runs after k rounds  $\Rightarrow k \leq \log_d(\frac{n}{M})$ .
- We have  $O(\frac{n}{B})$  block-transfers per round.
- $d \approx \frac{M}{B} 1$ .
- $\Rightarrow$  Total # block transfers is proportional to

$$\log_d(\frac{n}{M}) \cdot \frac{n}{B} \in O(\log_{M/B}(\frac{n}{M}) \cdot \frac{n}{B})$$

One can prove lower bounds in the external memory model:

We require  $\Omega(\log_{M/B}(\frac{n}{M}) \cdot \frac{n}{B})$  block transfers in any comparison-based sorting algorithm.

(The proof is beyond the scope of the course.)

d-way mergesort is optimal (up to constant factors)!

#### Outline

- External Memory
  - Motivation
  - Stream-based algorithms
  - External sorting
  - External Dictionaries
  - 2-4 Trees
  - a-b-Trees
  - B-Trees

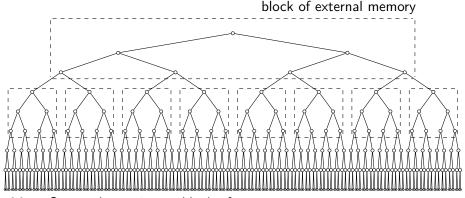
## Dictionaries in external memory

**Recall**: Dictionaries store *n* KVPs and support *search*, *insert* and *delete*.

- Recall: AVL-trees were optimal in time and space in RAM model
- $\Theta(\log n)$  run-time  $\Rightarrow O(\log n)$  block transfers per operation
- But: Inserts happen at varying locations of the tree.
  - → nearby nodes are unlikely to be on the same block
  - $\rightsquigarrow$  typically  $\Theta(\log n)$  block transfers per operation
- We would like to have fewer block transfers.

**Better solution**: design a tree-structure that *guarantees* that many nodes on search-paths are within one block.

#### Idealized structure



Idea: Store subtrees in one block of memory.

- ullet If block can hold subtree of size b-1, then block covers height  $\log b$
- $\Rightarrow$  Search-path hits  $\frac{\Theta(\log n)}{\log b}$  blocks  $\Rightarrow \Theta(\log_b n)$  block-transfers
  - Block acts as one node of a multiway-tree (b-1 KVPs, b subtrees)

#### Towards B-trees

- Idea: Define multiway-tree
  - ► One node stores many KVPs
  - ▶ Always true: b-1 KVPs  $\Leftrightarrow b$  subtrees
- To allow insert/delete, we permit varying numbers of KVPs in nodes
- This gives much smaller height than for AVL-trees
  - ⇒ fewer block transfers
- Study first one special case: 2-4-trees
  - ► Also useful for dictionaries in internal memory
  - May be faster than AVL-trees even in internal memory

#### Outline

#### 11 External Memory

- Motivation
- Stream-based algorithms
- External sorting
- External Dictionaries
- 2-4 Trees
- a-b-Trees
- B-Trees

#### 2-4 Trees

#### Structural property: Every node is either

- 1-node: one KVP and two subtrees (possibly empty), or
- 2-node: two KVPs and three subtrees (possibly empty), or
- 3-node: three KVPs and four subtrees (possibly empty).

**Order property:** The keys at a node are between the keys in the subtrees.

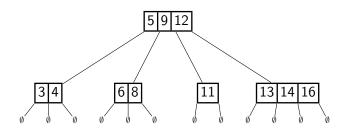
• With this, search is much like in binary search trees.



Another structural property: All empty subtrees are at the same level.

• This is important to ensure small height.

## 2-4 Tree example

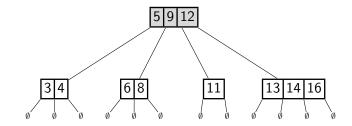


- Empty trees do not count towards height
  - ► This tree has height 1
- Easy to show: Height is in  $O(\log n)$ , where n = # KVPs.
  - ▶ Layer i has at least  $2^i$  nodes for i = 0, ..., h
  - ► Each node has at least one KVP.

## 2-4 Tree Operations

- Search is similar to BST:
  - ► Compare search-key to keys at node
  - ▶ If not found, recurse in appropriate subtree

**Example**: search(15) not found



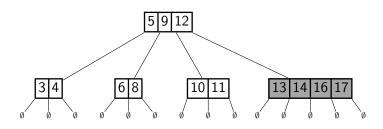
## 2-4 Tree operations

```
24Tree::search(k, v \leftarrow root, p \leftarrow NIL)
k: key to search, v: node where we search, p: parent of v
       if v represents empty subtree
1.
             return "not found, would be in p"
    Let \langle T_0, k_1, \dots, k_d, T_d \rangle be key-subtree list at v
4.
     if k > k_1
             i \leftarrow \text{maximal index such that } k_i \leq k
5.
            if k_i = k
6.
                  return KVP at ki
7.
             else 24Tree::search(k, T_i, v)
8.
9.
       else 24Tree::search(k, T_0, v)
```

#### Insertion in a 2-4 tree

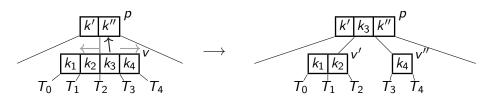
#### Example: insert(17)

- Do 24Tree::search and add key and empty subtree at leaf.
- If the leaf had room then we are done.
- Else **overflow**: More keys/subtrees than permitted.
- Resolve overflow by node splitting.



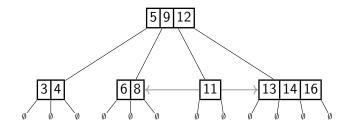
### 2-4 Tree operations

```
24Tree::insert(k)
       v \leftarrow 24Tree::search(k) // leaf where k should be
        Add k and an empty subtree in key-subtree-list of v
3.
        while v has 4 keys (overflow \rightsquigarrow node split)
              Let \langle T_0, k_1, \dots, k_4, T_4 \rangle be key-subtree list at v
4.
5.
              if (v has no parent) create a parent of v without KVPs
              p \leftarrow \text{parent of } v
6
              v' \leftarrow new node with keys k_1, k_2 and subtrees T_0, T_1, T_2
7.
              v'' \leftarrow new node with key k_4 and subtrees T_3, T_4
8
              Replace \langle v \rangle by \langle v', k_3, v'' \rangle in key-subtree-list of p
9
10.
              v \leftarrow p
```



#### Towards 2-4 Tree Deletion

- For deletion, we symmetrically will have to handle underflow (too few keys/subtrees)
- Crucial ingredient for this: immediate sibling

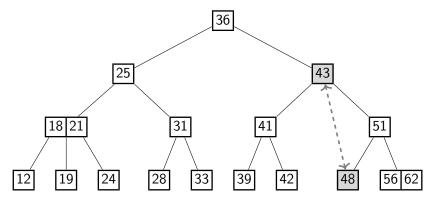


Observe: Any node except the root has an immediate sibling.

#### 2-4 Tree Deletion

#### Example:

- 24Tree::search, then trade with successor if KVP is not at a leaf.
- If underflow:
  - ► If immediate sibling has extras, rotate/transfer
  - ► Else **node merge** (this affects the parent!)



#### Deletion from a 2-4 Tree

```
24Tree::delete(k)
      v \leftarrow 24Tree::search(k) // node containing k
2. if v is not leaf
3.
            swap k with its successor k' and v with leaf containing k'
4.
      delete k and one empty subtree in v
5.
      while v has 0 keys (underflow)
6.
            if parent p of v is NIL, delete v and break
7.
           if v has immediate sibling u with 2 or more keys (transfer/rotate)
8.
                 transfer the key of u that is nearest to v to p
9.
                 transfer the key of p between u and v to v
                 transfer the subtree of u that is nearest to v to v
10.
                 break
11.
12.
           else (merge & repeat)
                 u \leftarrow \text{immediate sibling of } v
13.
                 transfer the key of p between u and v to u
14
15.
                 transfer the subtree of v to u
16.
                 delete node v and set v \leftarrow p
```

## 2-4 Tree summary

- A 2-4 tree has height  $O(\log n)$ 
  - ▶ In internal memory, all operations have run-time  $O(\log n)$ .
  - ► This is no better than AVL-trees in theory. (Though 2-4-trees are faster than AVL-trees in practice, especially when converted to binary search trees called *red-black trees*. No details.)
- A 2-4 tree has height  $\Omega(\log n)$ 
  - ► Level *i* contains at most 4<sup>*i*</sup> nodes
  - ► Each node contains at most 3 KVPs
- So not significantly better than AVL-trees w.r.t. block transfers.
- But we can generalize the concept to decrease the height.

#### Outline

#### 11 External Memory

- Motivation
- Stream-based algorithms
- External sorting
- External Dictionaries
- 2-4 Trees
- a-b-Trees
- B-Trees

#### *a-b*-Trees

A 2-4 tree is an a-b-tree for a = 2 and b = 4.

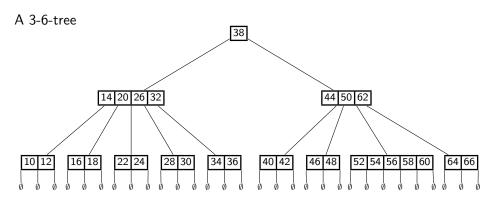
#### An a-b-tree satisfies:

- Each node has at least *a* subtrees, unless it is the root. The root has at least 2 subtrees.
- Each node has at most b subtrees.
- A node has d subtrees  $\Leftrightarrow$  it stores d-1 KVPs
- Empty subtrees are at the same level.
- The keys in the node are between the keys in the corresponding subtrees.

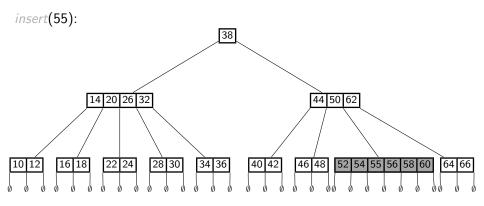
Requirement: 
$$a \leq \lceil b/2 \rceil = \lfloor (b+1)/2 \rfloor$$
.

search, insert, delete then work just like for 2-4 trees, after re-defining underflow/overflow to consider the above constraints.

### *a-b*-tree example



## a-b-tree insertion

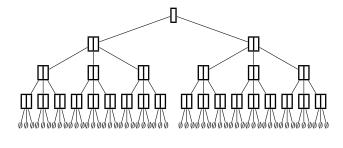


- Overflow now means b keys (and b+1 subtrees)
- Node split  $\Rightarrow$  new nodes have  $\geq \lfloor (b-1)/2 \rfloor$  keys
- Since we required  $a \le \lfloor (b+1)/2 \rfloor$ , this is  $\ge a-1$  keys as required.

### Height of an a-b-tree

**Recall:** n = numbers of KVPs (not the number of nodes) What is smallest possible number of KVPs in an a-b-tree of height-h?

Level	Nodes
0	$\geq 1$
1	$\geq 2$
2	$\geq 2a$
3	$\geq 2a^2$
	• • •
h	$\geq 2a^{h-1}$



# nodes 
$$\geq \underbrace{1}_{\text{root: } \geq 1 \text{ KVP}} + \underbrace{\sum_{i=0}^{h-1} 2a^{i}}_{\text{others: } \geq a-1 \text{ KVPs}}$$

$$n = \# \text{ KVPs} \geq 1 + (a-1) \sum_{i=0}^{h-1} 2a^{i} = 1 + 2(a-1) \frac{a^{h}}{a-1} = 1 + 2a^{h}$$

Therefore the height of an a-b-tree is  $O(\log_a(n)) = O(\log n / \log a)$ .

### a-b-trees as implementations of dictionaries

**Analysis** (if entire *a-b*-tree is stored in internal memory):

- search, insert, and delete each requires visiting  $\Theta(height)$  nodes
- Height is  $O(\log n/\log a)$ .
- Recall:  $a \leq \lceil b/2 \rceil$  required for insert and delete
- $\Rightarrow$  choose  $a = \lceil b/2 \rceil$  to minimize the height.
  - Work at node can be done in  $O(\log b)$  time.

Total cost: 
$$O\left(\frac{\log n}{\log a} \cdot (\log b)\right) = O(\log n \cdot \frac{\log b}{\log b - 1}) = O(\log n)$$

This is still no better than AVL-trees.

The main motivation for a-b-trees is external memory.

#### Outline

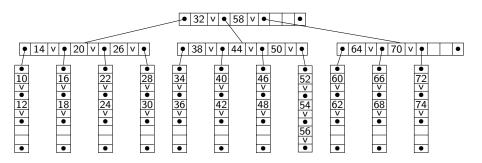
### 11 External Memory

- Motivation
- Stream-based algorithms
- External sorting
- External Dictionaries
- 2-4 Trees
- a-b-Trees
- B-Trees

#### B-trees

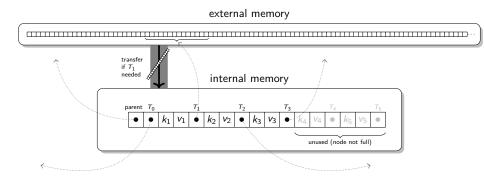
A B-tree is an a-b-tree tailored to the external memory model.

- Every node is one block of memory (of size *B*).
- b is chosen maximally such that a node with b-1 KVPs (hence b-1 value-references and b subtree-references) fits into a block. b is called the **order** of the B-tree. Typically  $b \in \Theta(B)$ .
- a is set to be  $\lceil b/2 \rceil$  as before.



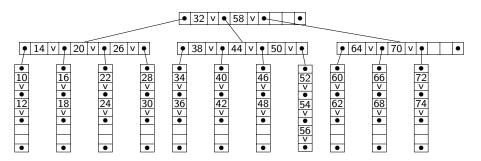
## B-tree in external memory

Close-up on one node in one block:



In this example: 17 computer-words fit into one block, so the *B*-tree can have order 6.

### B-tree analysis



- search, insert, and delete each requires visiting  $\Theta(height)$  nodes
- ullet Work within a node is done in internal memory  $\Rightarrow$  no block-transfer.
- The height is  $\Theta(\log_a n) = \Theta(\log_B n)$  (presuming  $a = \lceil b/2 \rceil \in \Theta(B)$ )

So all operations require  $\Theta(\log_B n)$  block transfers.

## B-tree summary

- All operations require  $\Theta(\log_B n)$  block transfers. This is asymptotically optimal.
- In practice, height is a small constant.
  - Say  $n = 2^{50}$ , and  $B = 2^{15}$ . So roughly  $b = 2^{14}$ ,  $a = 2^{13}$ .
  - ▶ *B*-tree of height 4 would have  $\geq 1 + 2a^4 > 2^{50}$  KVPs.
  - ► So height is 3.
- There are some variations that are even better in practice (no details).
- B-trees are hugely important for storing data bases (→ cs448)