XML : New Challenges and Opportunities for Database Research

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Road Map

- Introduction: Basic understanding of XML
- Case Study: Microarray gene expr data
- Challenges and Proposed Solutions
  - XML to RDB Mapping
  - Indexing XML data for Path Queries
    - XISS/Numbering Scheme and Path Joins
  - Selectivity Estimation
- Concluding Remarks

HTML vs. XML

- **HTML tags are mostly for formatting purpose. How something should look.**
  - **Most XML documents are *exchanged* by applications that do not display them for human consumption.**
- **HTML tags are not informative about the contents.**
  - **XML tags are *self-describing* and can be *tailored* for different categories of applications.**
- **HTML files are too forgiving; not suitable for automatic processing.**
  - **XML data is *well-formed* and its *validity* may be checked by applications or processors.**

Extensible and Self-describing

- **No preset semantics for any XML tag**
  - Different semantic layers are supposed to be built atop XML data.
  - Create your own *markup language*. (E.g., GEML, MAML)
- ***eXensible*: You can create your own *tags*.**

```
<author>Bongki Moon</author>
<picture filename="tiger.jpg" />
<pattern name="XYZ">
    <reporter active_sequence="TCTCACTGGTCA">
    ….
    </reporter>
    <position x="0.3", y="0.5" />
</pattern>
```

Well-formed *but* Semi-structured

- ***Well-formedness***
  - Every XML document has a root element
  - Matching opening-closing tags; properly nested
  - An attribute can occur at most once in an opening tag, and its value must be provided.
- ***Tree-structured***
  - Not as structured as relational databases
  - ***Need a special-purpose DBMS for XML data?***

More Specifics of XML

- Elements are ordered; attributes are *not* ordered
- *String* is one and only primitive data type in XML; complex data types can be defined in *XML Schema*
- DTD is a set of rules that specify which elements and attributes are allowed in a custom markup language.

```
<!DOCTYPE bioinfo_bib [
    <!ELEMENT bioinfo_bib (article*)>
    <!ELEMENT article (author+,title,source)>
    <!ELEMENT author (#PCDATA)>
    <!ELEMENT author email_address>
    ....
]>
```

- DTD defines the structural relationship between elements.
- A standard maintained by the WWW Consortium (www.w3c.org/XML)

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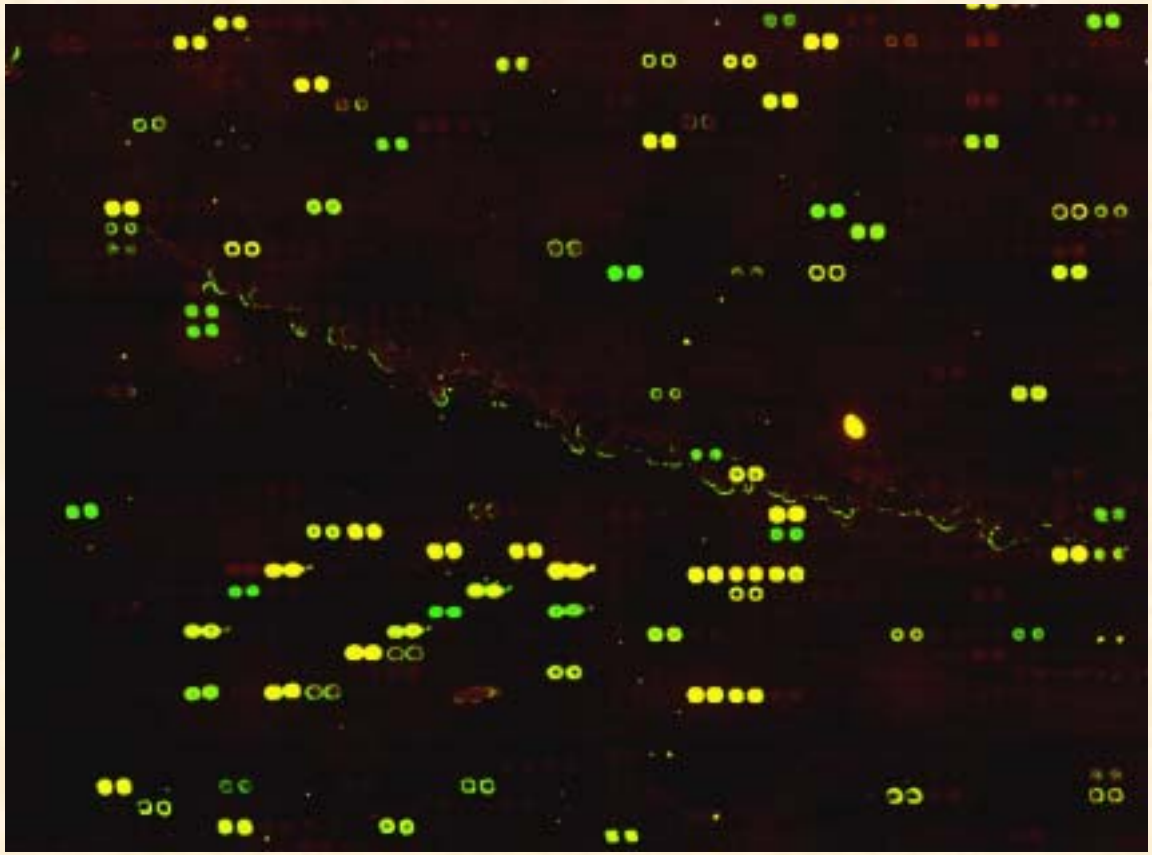
Case Study: *Microarray Data*

- **DNA Microarray technology**
  - **Many thousands of DNA samples are arrayed on a glass slide, and competitively hybridized**
  - **Simultaneously monitor the expression levels of thousands of genes**
  - **Enormous opportunities to identify target genes for drug development and cancer classification**

A Hybridized Mouse Microarray



Courtesy of Dr. James Hoying at Arizona Research Laboratories

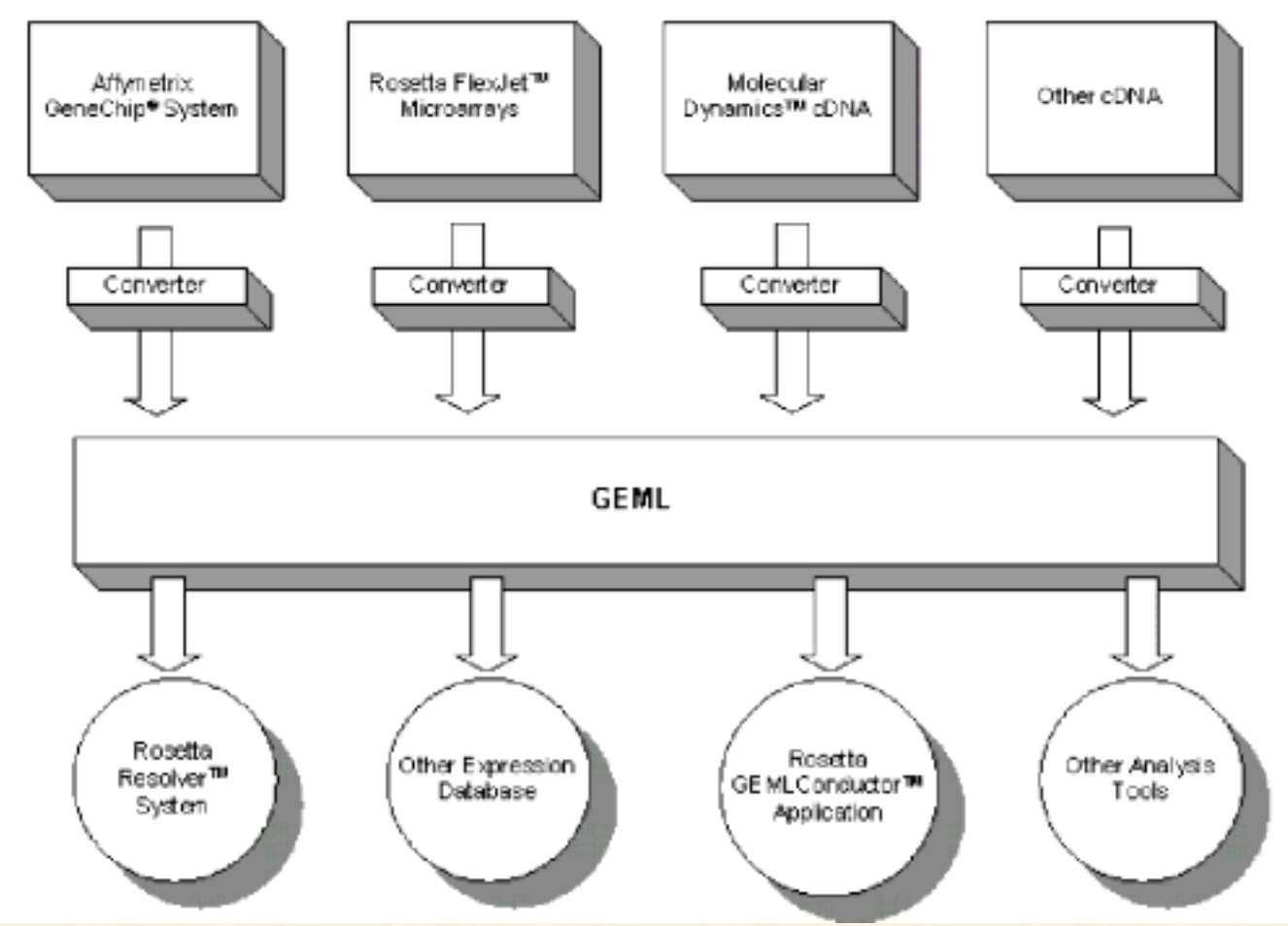
Issues and Approaches

- **Main challenges in establishing a public microarray gene expr database [Blazma 1999]**
  - **Annotation of experiments in a standardized and machine-readable way**
  - **Normalization procedures and standards enabling the comparison of data from different experiments and platforms**
- **Consensus emerged [MGED and MIAME, etc.]**
  - **Standards for storing and annotating data can be developed based on the *XML technology***

Markup Languages and Repositories

- To store data about *patterns, profiles and hybridization* for gene expression analysis
- MAML (MicroArray Markup Language)
  - MGED group (www.mged.org)
- GEML (Gene Expression Markup Language)
  - Rosetta Inphamatics (www.geml.org)
- Public repositories
  - GeneX (National Center for Genome Resources)
  - Gene Expression Omnibus (National Center for Biotechnology Information)
  - ArrayExpress (European Bioinformatics Institute)

Loading Gene Expr Data



By courtesy of ROSETTA Inphamatics

GEML Doc Type Definitions

- **GEML defines two Document Type Definitions: GEMLPattern.dtd and GEMLProfile.dtd.**
  - Pattern DTD **describes genes, reporters, and chip layout.**
  - Profile DTD **describes gene expression data, cell, treatment, and hybridization information.**

GEMLPattern.dtd

```
<?xml version="1.0" standalone="no"?>
<!DOCTYPE project SYSTEM "GEMLPattern.dtd">
<project name="Hsapiens-421205160837"
   date="07-12-1999 12:43:48"
   by="jzsmith"
   company="JZSmith Technologies" >
   <pattern name="Hsapiens-421205160837">
      <reporter
        name="XV186450"
        systematic_name="XV186450"
        active_sequence="TCTCACTGGTCAGGGGTCTCTCCC"
        start_coord="159">
        <feature number="6878">
         <position x="0.3333" y="0.508374" units="inches"/>
           </feature>
              <gene primary_name="XV186450"
                systematic_name="XV186450" >
                <accession database="n/a" id="XV186520" />
                </gene>
      </reporter>
      <reporter
        name="T89593"
        systematic_name="T89593"
        active_sequence="TACAGTGTCAGAATTAACTGTAGTC"
        start_coord="201">
        <feature number="6879">
                <position x="0.340707" y="0.508374" units="inches" />
                </feature>
                <gene primary_name="T89593" systematic_name="T89593" >
                  <accession database="n/a" id="T89593" />
                </gene>
                  </reporter>
      <!-- Total Number of Reporters: 2 -->
   </pattern>
   <printing date="07-12-1999 12:43:48" printer="2" type="INKJET"
pattern_name="Hsapiens-421205160837" >
      <chip barcode="JZS123456781" />
      <chip barcode="JZS123456782" />
      <chip barcode="JZS123456783" />
      <chip barcode="JZS123456784" />
   </printing>

</project>
```

By courtesy of ROSETTA Inphamatics

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Challenges in XML Research

- **Storing and Publishing XML**
  - Use Relational DBMS to store XML data?
  - Publish relational data in XML format for exchange
  - Store and access Versioned XML data
- **Indexing and Querying XML**
  - Fast access to XML data via path expressions
    - XPath and XQuery [W3C]
  - XML query optimization, selectivity estimation

Work in Progress

- **RDB mapping and XML publication**
  - Edge table [INRIA 1999]
  - Inlining and Outer union [VLDB'99 & VLDB'00]
  - XRel path-based storage [TOIT'01]
  - Cost-based storage mapping [ICDE'02]
- **Indexing for Path Queries**
  - Index Fabric: Block-structured Patricia [VLDB'01]
  - XISS and Path Joins [Li & Moon, VLDB'01]
- **Selectivity estimation**
  - Path tree and Markov table [Wisc, VLDB'01]
  - Position histogram [Michigan, EDBT'02]
- **XML versioning**
  - UBCC clustering [UCLA & UCR, VLDB'01, EDBT'02]

XML to RDB Mapping

- **Edge Table [INRIA 1999]**
  - Map each <parent, child> pair to a tuple in Edge(source_id, ordinal,name,flag,target
  - Disadvantages
    - Storage overhead due to redundant data
    - Too many self-joins are required
- **DTD Graph and Inlining [VLDB'99]**
  - Build a DTD graph from a simplified DTD
  - DFS traveral to create (potentially too many) relational tables
  - Avoid fragmentation problem by inlining descendants of an element into a single relation

XML to RDB Mapping

- **XRel: path-based storage [TOIT'01]**
  - Path Table stores distinct (root-to-any) paths
  - Element Table associates each path with a region where the instances of a path appear
- **Lego: cost-based mapping [ICDE'02]**
  - Transformations at the XML Schema level
  - Apply a greedy heuristic to find an efficient one
    - Feed a relational query optimizer with a relational schema and statistics
    - Compute the expected cost of computing queries

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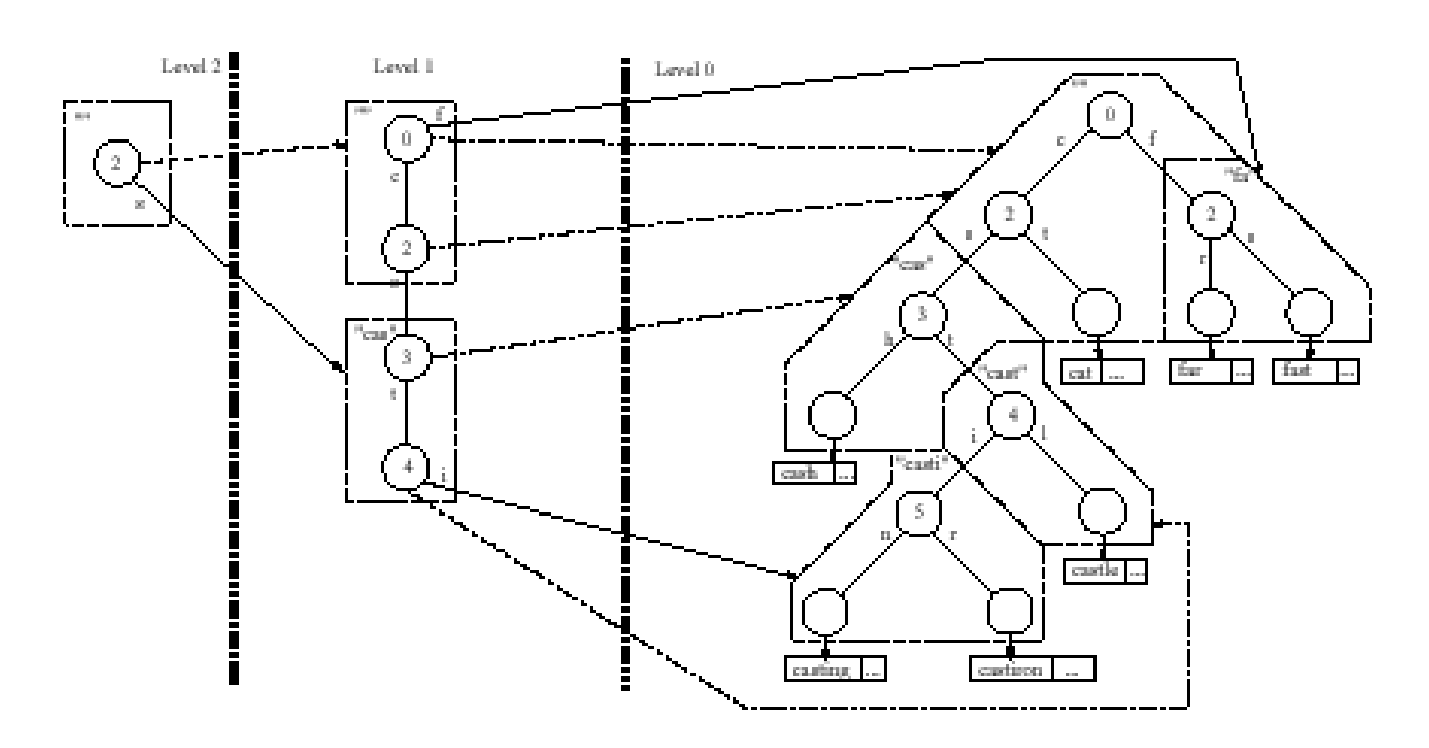
Query by Path Expressions

- **Path expressions to navigate through and retrieve XML data**
  - **Q1: /chapter//figure[@caption="Tree Frogs"]**
  - **Q2: $(E_1/E_2)^+/E_3/((E_4[@A=v])|(E_5//E_6))$**
    - **Kleene-closure is not in XQuery 1.0.**
- **Common Feature of XML Query Languages**
  - **Lorel, XML-QL, XML-GL, XPath, etc.**
  - **XQuery working draft [W3C;Feb. 2001]**

Indexing for Path Queries

- **Index Fabric [VLDB'01]**
  - All (root-to-leaf) paths are encoded as strings and inserted into a Patricia
  - Maintain the Patricia as a block-structured tree like B^+-tree; High fan-out can be achieved
  - A sub-path match query is posed as a path query with a wildcard as a prefix
- **Disadvanteges?**
  - A sub-path match query is posed a path query with a ***wildcard as a prefix***
    - It could be slow ***without suffixes*** of paths in the index
  - No guarantee of the minimum storage utilization

Example: 3-level index fabric



RightOrder Inc., 2001

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XISS and Path Joins [VLDB'01]

- Design a numbering scheme
  - Based on *Extended Preorder*
  - Determine ancestor-descendant relationship
- Propose *Path-Join* algorithms
  - Conventional tree traversal is slow
  - Join algorithms to avoid tree traversal
- Design indexing and storage structures
  - *XISS*: Element index, attribute index, structure index, etc.

Numbering Scheme

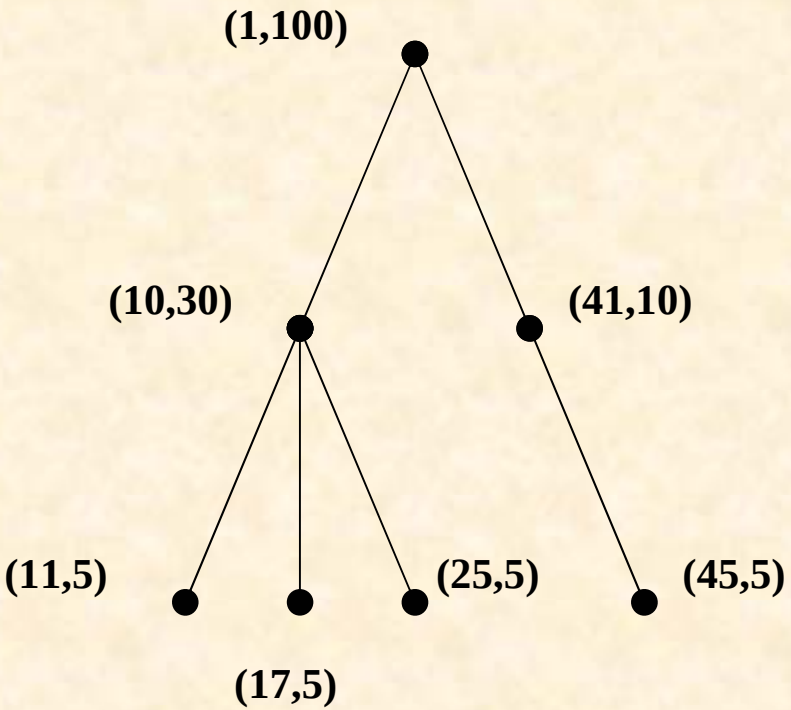
- XML objects are modeled by a tree structure
  - Nodes are XML elements and attributes
  - Parent-child represents nesting between objects
- To process path expression queries
  - (e.g.) chapter3/section, chapter3//figure
  - Conventional approach : traverse XML trees
  - New Approach :
    - Collect two object sets
    - Determine A-D relationship between objects

Extended Preorder

- Annotate a node with a pair of <order,size>
  - For Y and its parent X,
    - order(X) < order(Y) and
    - order(Y)+size(Y) ≤ order(X)+size(X)
  - For sibling X and Y, if X is before Y in preorder,
    - order(X)+size(X) < order(Y)
- Lemma: X is an ancestor of Y iff

  order(X) < order(Y) ≤ order(X)+size(X)
- Size can be pre-allocated to accommodate future insertion.

Extended Preorder: Examples

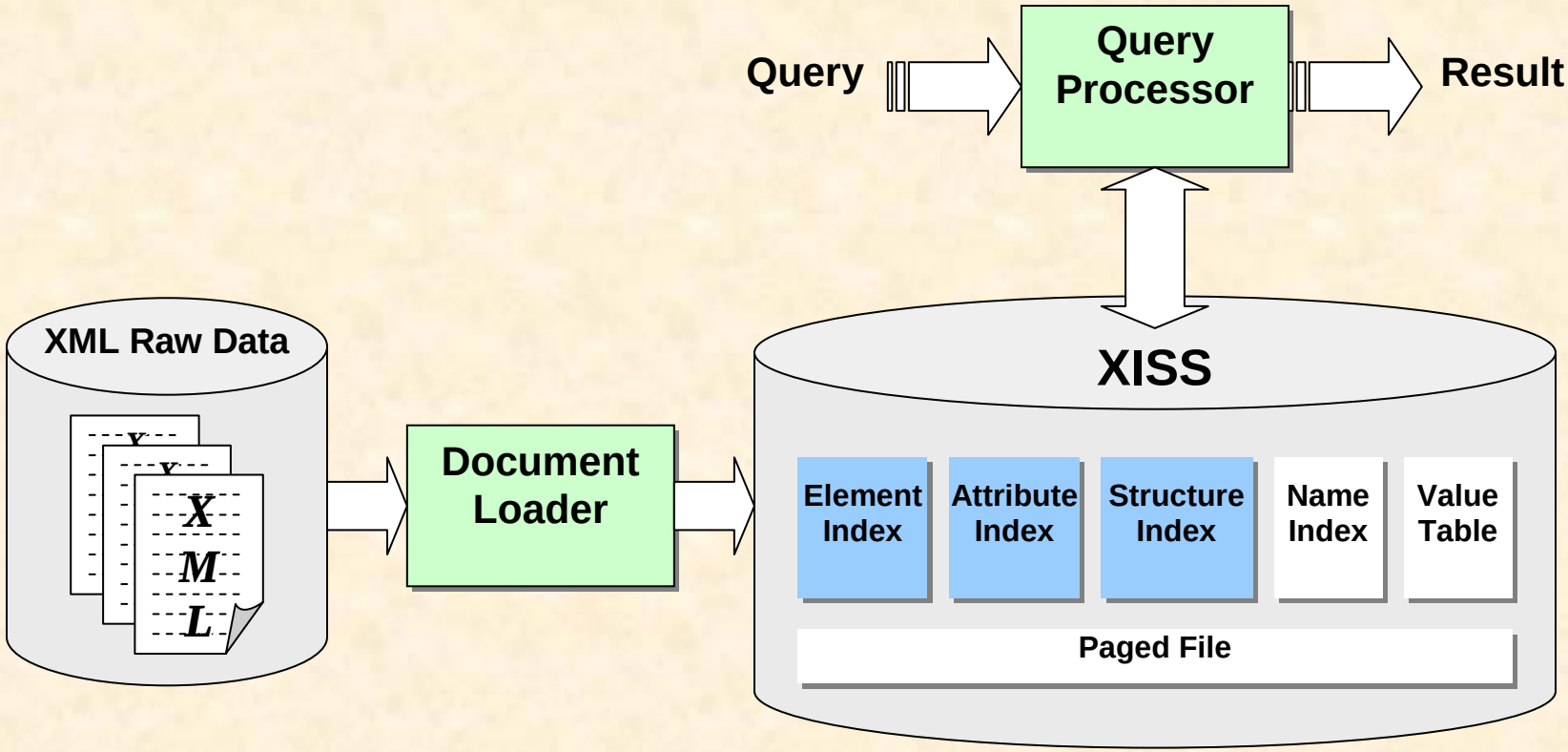


- (1,100) is an ancestor of (17,5)
  - 1 < 17
  - 17 < 1+100
- (10,30) is not an ancestor of (45,5)
  - 45 > 10+30

Index and Data Organization

- **Operations to support**
  - For a name string, find a list of elements (or attributes) having the same name string.
  - For a given object, find its parent and children.
- **Two supplementary structures**
  - ***Name index*** maps a name string to **nid**
    - Minimize storage and computational overhead
    - Implemented as a B^+-tree
  - ***Value table*** stores all string values

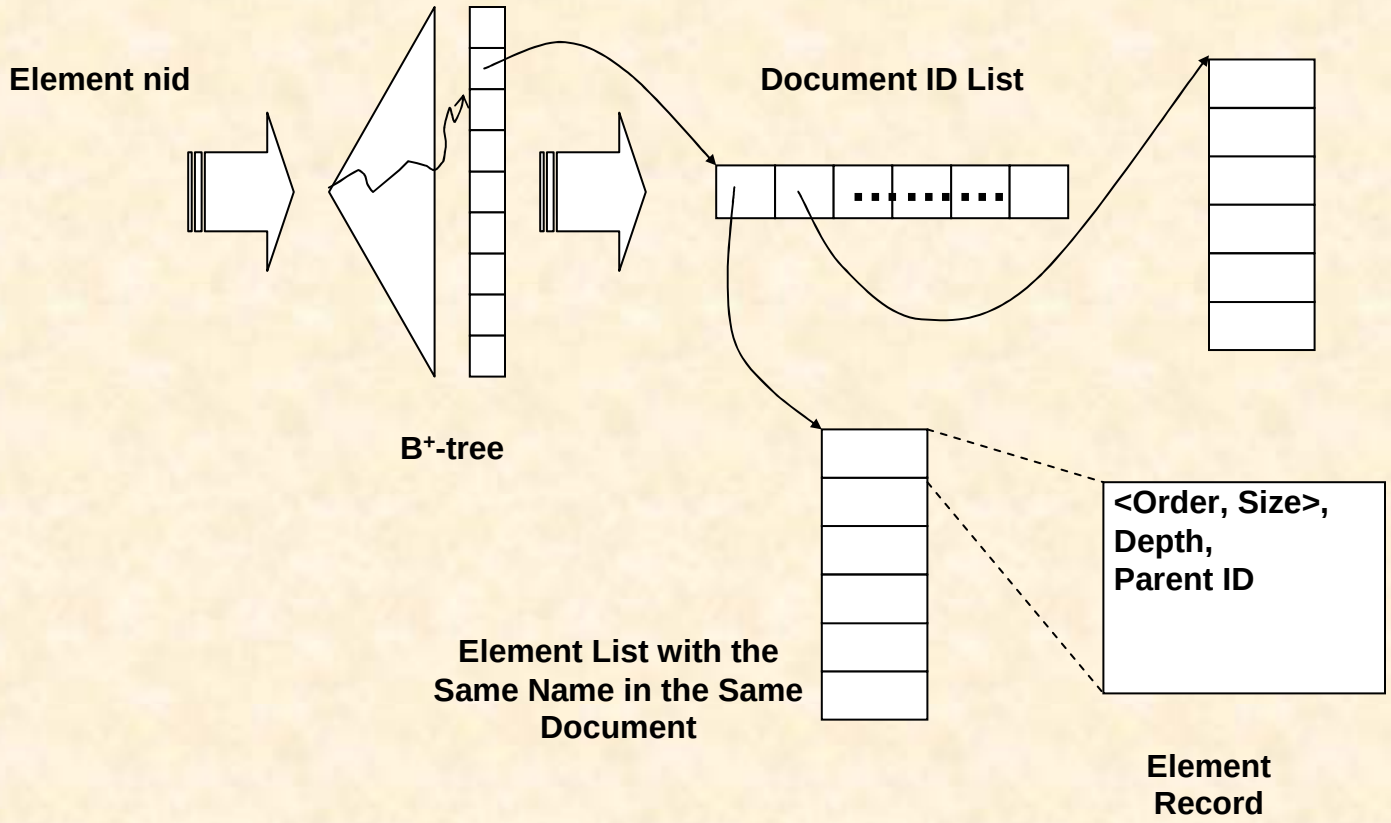
XISS Structure Overview



Element and Attribute Index

- Element Index maps nid to a list of element records grouped by did (document id).
  - Implemented as a B^+-tree
  - An element record is fixed-length containing:
    - <order,size>, depth, parent id
- Quickly find all elements having the same name string.
- Attribute Index is identical to E. index except
  - vid (value id) to attribute value in the Value Table.

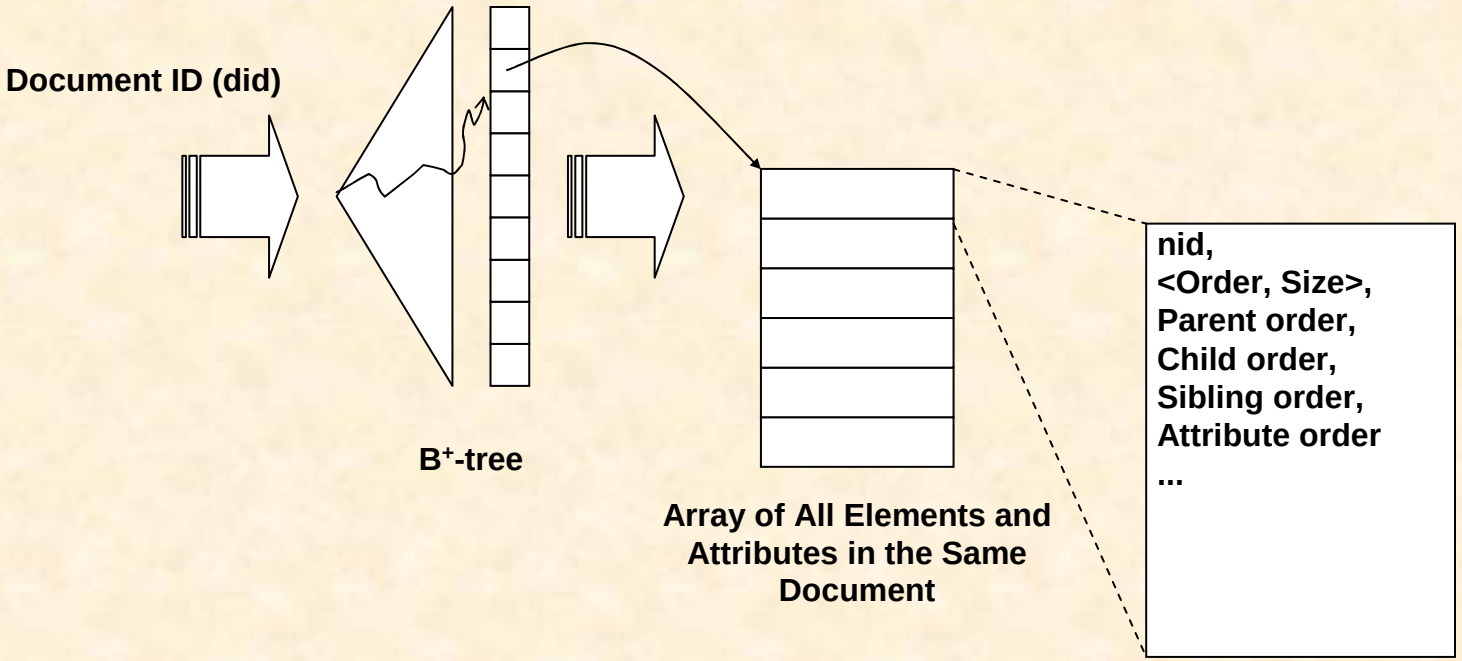
Element Index: illustration



Structure Index

- Structure Index maps did to a list of element and attribute records.
  - Implemented as a B^+-tree
  - Each record is fixed-length containing:
    - nid, <order,size>, parent-order, first-child-order, first-attribute-order, etc.
- Quickly locate an object record using did and nid

Structure Index: illustration



Path Expression Queries

Q1: document("*.xml")//chapter//figure[@caption="Tree Frogs"]

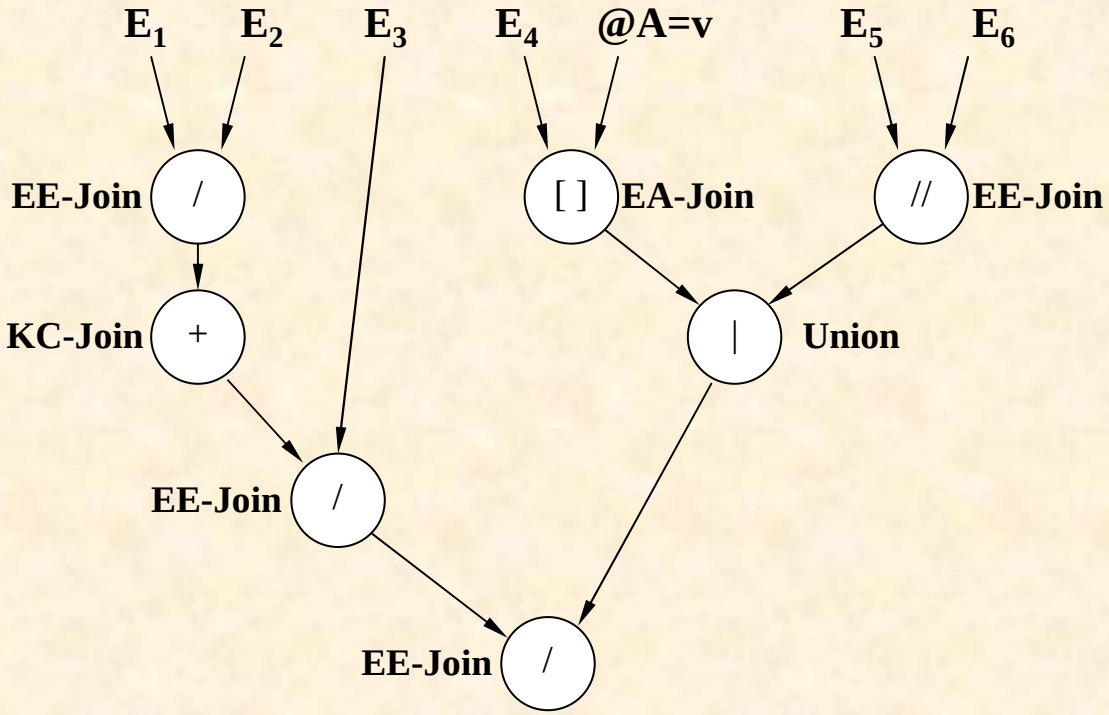
- **Conventional Approaches [McHugh, VLDB'99]**
  - **Top-Down Traversal**
    - Check all downward paths from **chapter**
  - **Bottom-Up Traversal**
    - Check all upward paths from **figure** with **@caption="Tree Frogs"**
  - **Hybrid**
    - Meeting in the middle of a path

Path-Join Algorithms

- **Apply Path-Join algorithms to a sub-expression**
  - **A single element or attribute**
    - Use the element index or attribute index
  - **A pair of element and attribute**
    - Use ***EA-Join*** algorithm
  - **A pair of two elements**
    - Use ***EE-Join*** algorithm
  - **A Kleene closure (+,*) of a subexpression**
    - Use ***KC-Join*** algorithm
  - **A Union of two subexpressions**
    - Merge two intermediate results and group by did

Path-Join Algorithms

- Decompose a path expression
  - Q2: $(E_1/E_2)^+/E_3/((E_4[@A=v])|(E_5//E_6))$



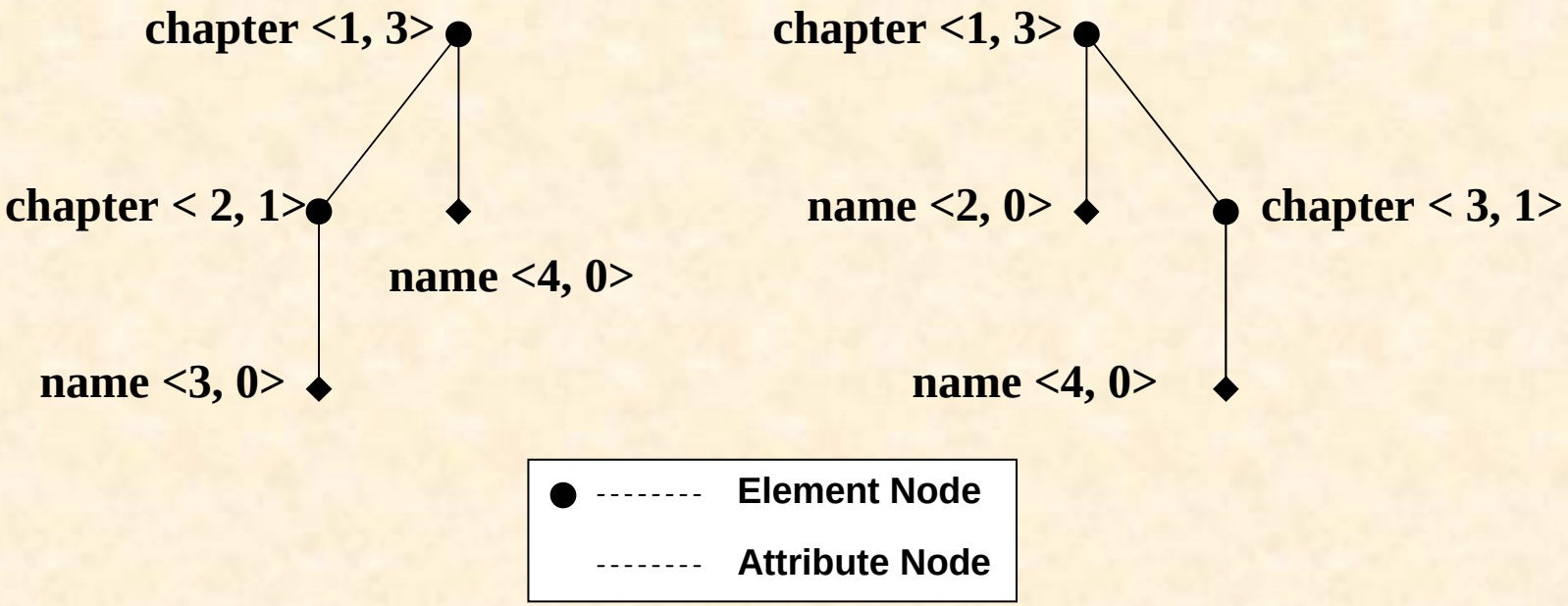
EA-Join Algorithm

- **Join an element set and an attribute set by A-D**
  - **(e.g.) figure[@caption="Tree Frogs"]**
- **Input**
  - **{.. E_i ..}, E_i is a set of elements from a document did**
  - **{.. A_j ..}, A_j is a set of attributes from a document did**
- **Output**
  - **A set of (*e*,*a*) pairs such that *e* is parent of *a***
- **Algorithm**

foreach E_i and A_j with the same did **do**
  foreach $e \in E_i$ **and** $a \in A_j$ **do**
    if (*e* is parent of *a*) **then** output (*e*,*a*);

EA-Join: single-scan requirement

- **Attribute nodes *before* their sibling elements in the order by the numbering scheme.**



EE-Join Algorithm

- **Join two element sets by A-D relationship**
  - **(e.g.) chapter//figure**
- **Input**
  - **{.. E_i ..} and {.. F_j ..}, E_i, F_j are a set of elements from the same document did**
- **Output**
  - **A set of (*e*,*f*) pairs such that *e* is an ancestor of *f***
- **Algorithm**

foreach E_i and F_j with the same did **do**

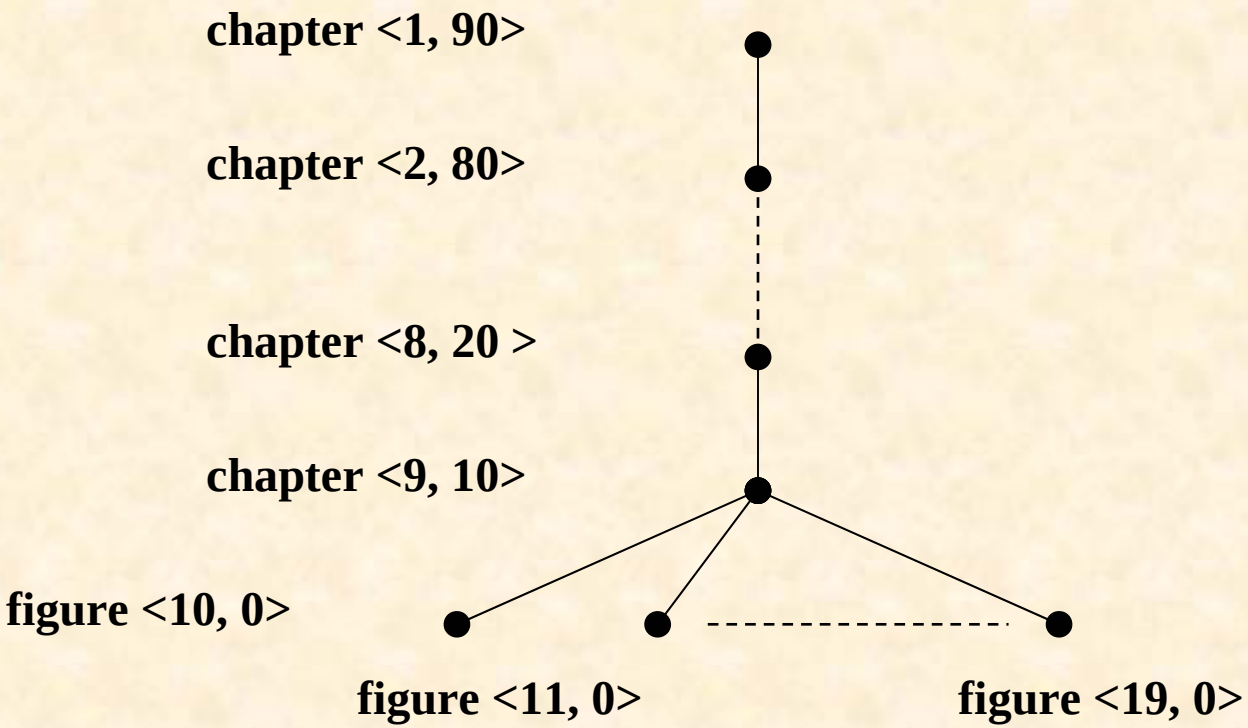
foreach $e \in E_i$ **and** $f \in F_j$ **do**

if (*e* is ancestor of *f*) **then** output (*e*,*f*);

EE-Join: Multiple Scans

- Use depth to process fixed-length path expression queries
  - (e.g.) chapter/*/*/figure
- Join by A-D relationship
  - Viewed as a join of a range set and a point set
    - Range: [order(chapter), order(chapter)+size(chapter)]
    - Point: order(figure)
  - Multiple scans are unavoidable
  - Still, very efficient for long or unknown-length paths

EE-Join: an extreme case



KC-Join Algorithm

- (e.g.) chapter*, figure+, chapter/chapter
- **Input**
  - {.. E_i ..}, E_i is a set of elements from a document did
- **Output**
  - A Kleene closure of {.. E_i ..}
- **Algorithm**

  $i = 1$; K_i = {.. E_i ..};

  repeat

  $i = i+1$; K_i = EE-Join(K_{i-1},K_1);

  until (K_i is empty)

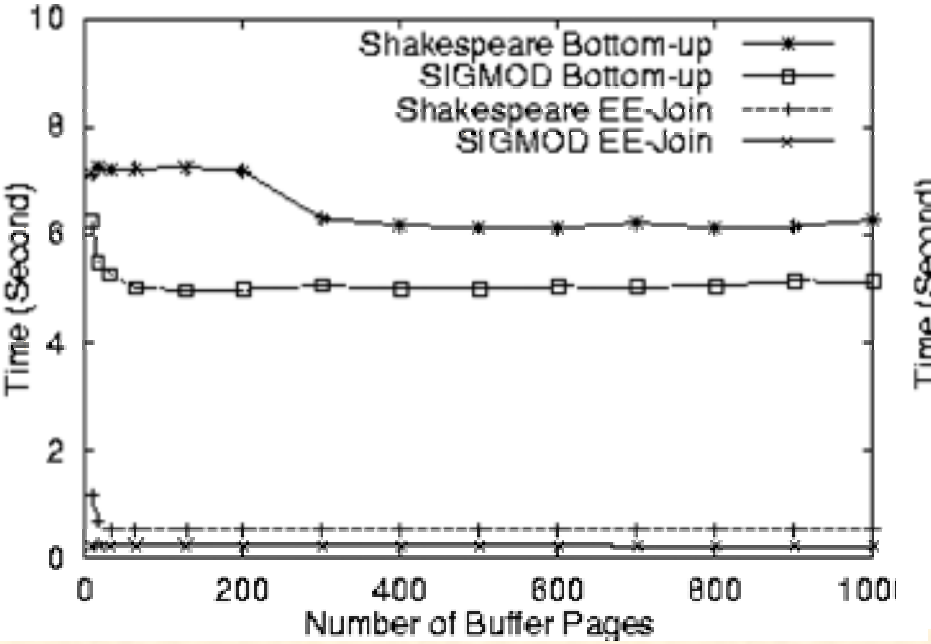
  output union of K_1, K_2, .. , K_{i-1};

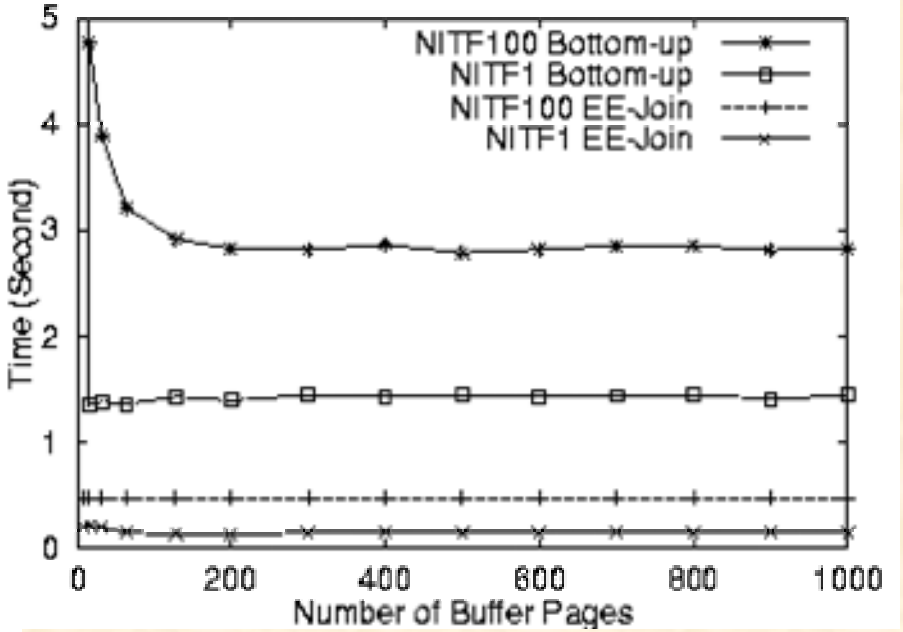
Experiment Settings

- XISS prototype system using C++ and GiST
- Sun Ultrasparc-II running Solaris 2.7
  - 256 MB Memory, 20 GB Disk w/ Ultra 10 EIDE
- Data sets
  - Real-world: Shakespeare's Plays, SIGMOD
    - Shakespeare's Plays: 327K(22) elements, 0(0) attributes
    - SIGMOD Record: 839K(47) elements, 4775(3) attributes
    - DBLP/conference: 2666K(29) elements, 199K(3) attributes
  - Synthetic: XML generator (IBM)
    - NITF (News Industry Text Format) as a DTD
      - NITF100: 63K(124) elements, 263K(142) attributes
      - NITF1: 38K(86) elements, 171K(106) attributes

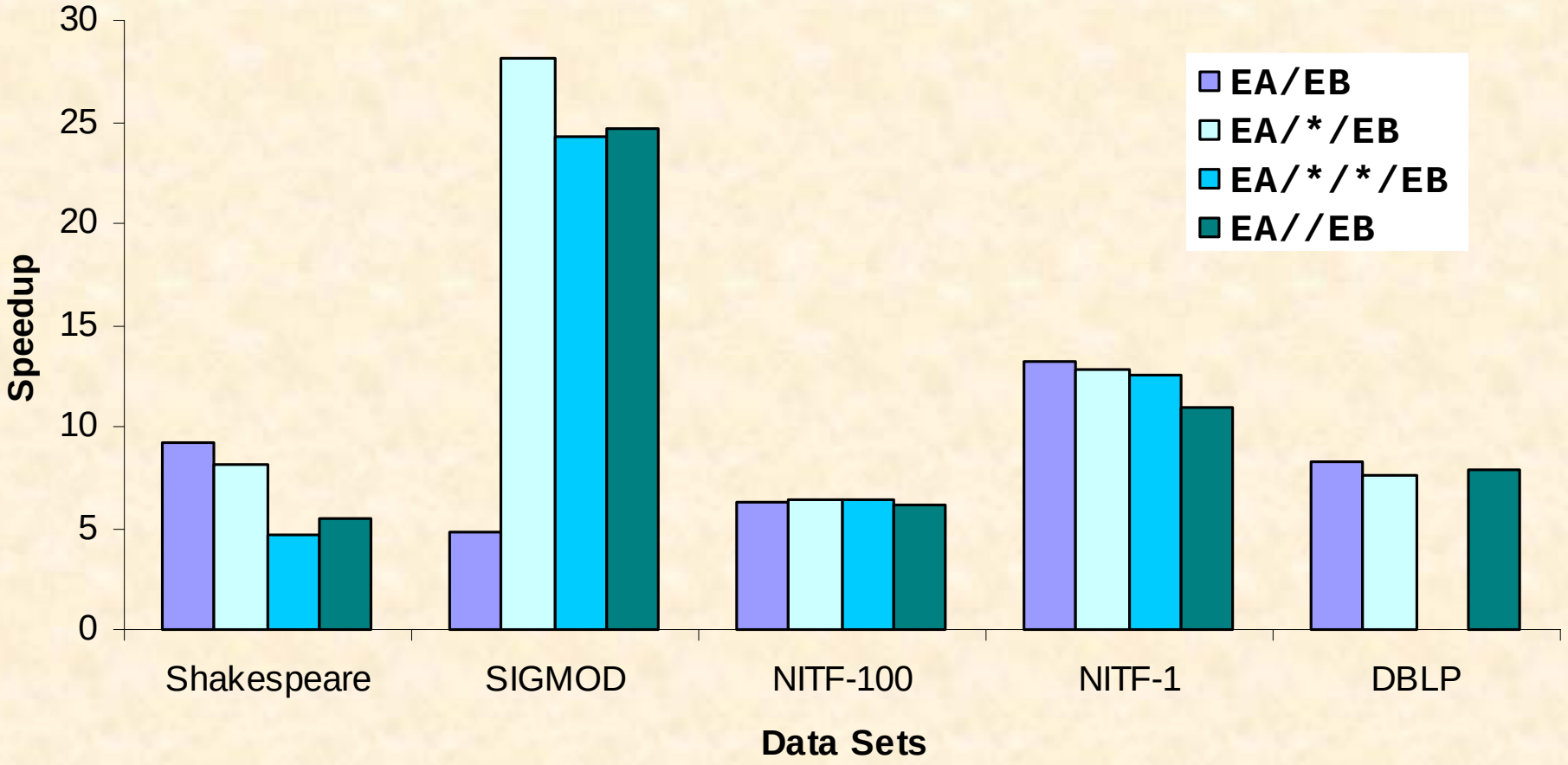
EE-Join Results

- Measured total elapsed time; IO time was dominant.
- An order of magnitude faster than bottom-up approaches.



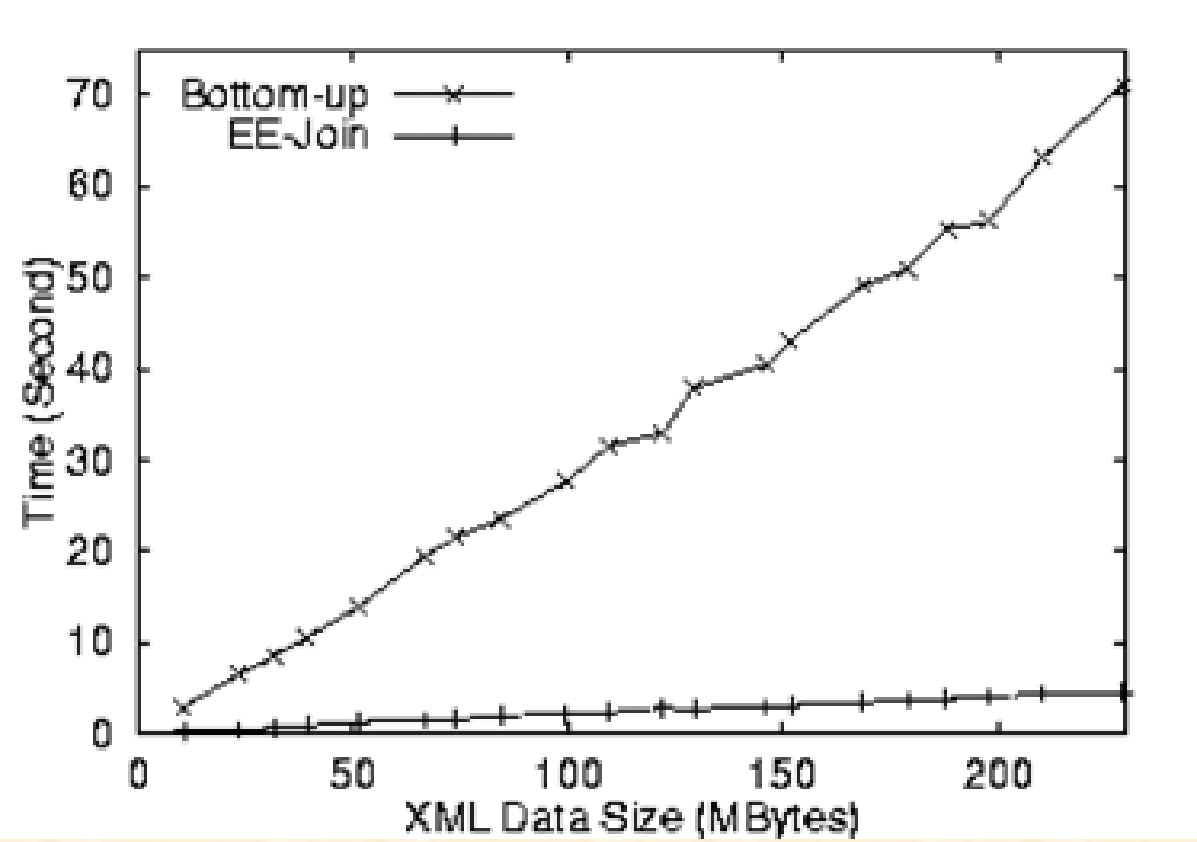


EE-Join: Speed-up



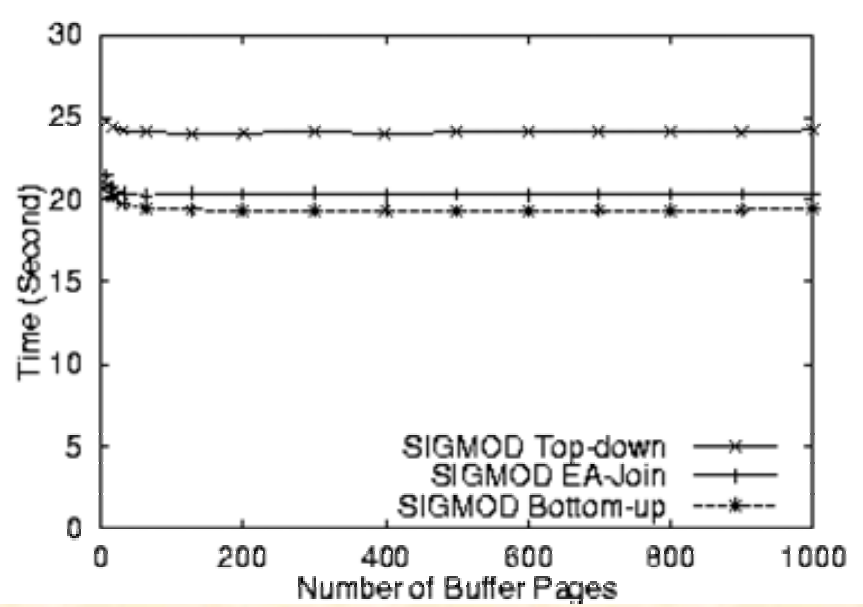
EE-Join: Scale-up

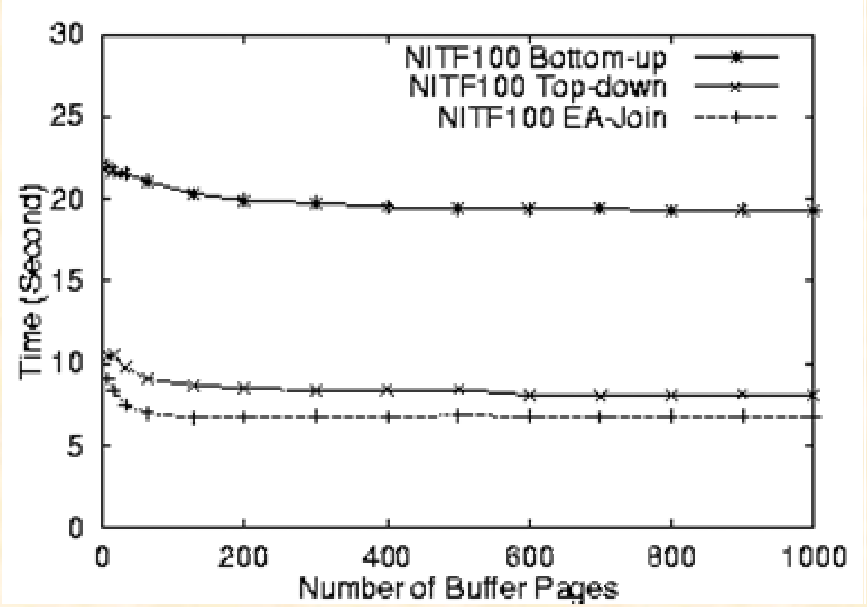
- **NITF data (229MB)**



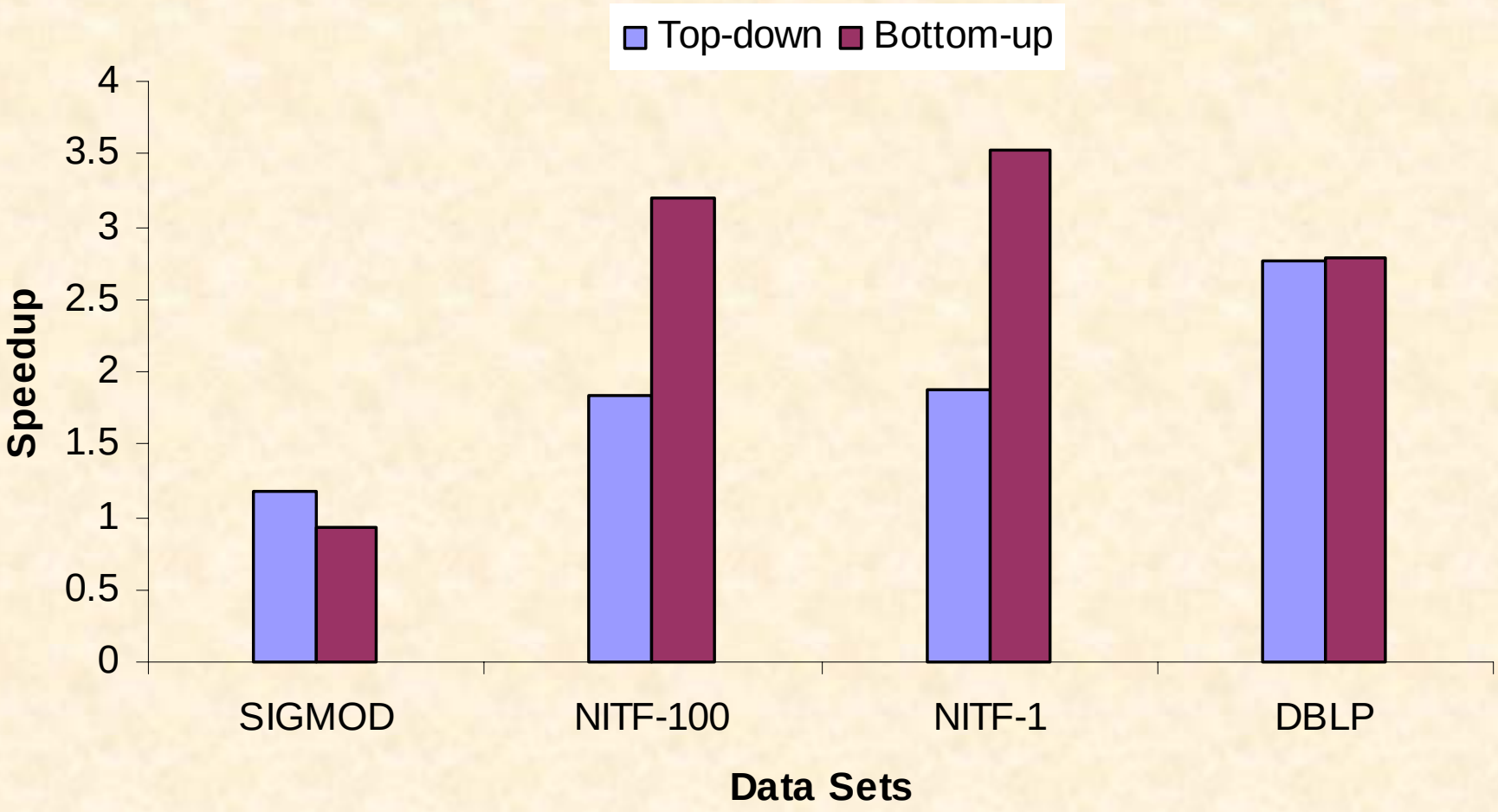
EA-Join Results

- Measured total elapsed time; IO time was dominant.
- SIGMOD data has a small number of attributes; bottom-up was slightly better than EA-Join.
- NTIF has much more attributes than elements.



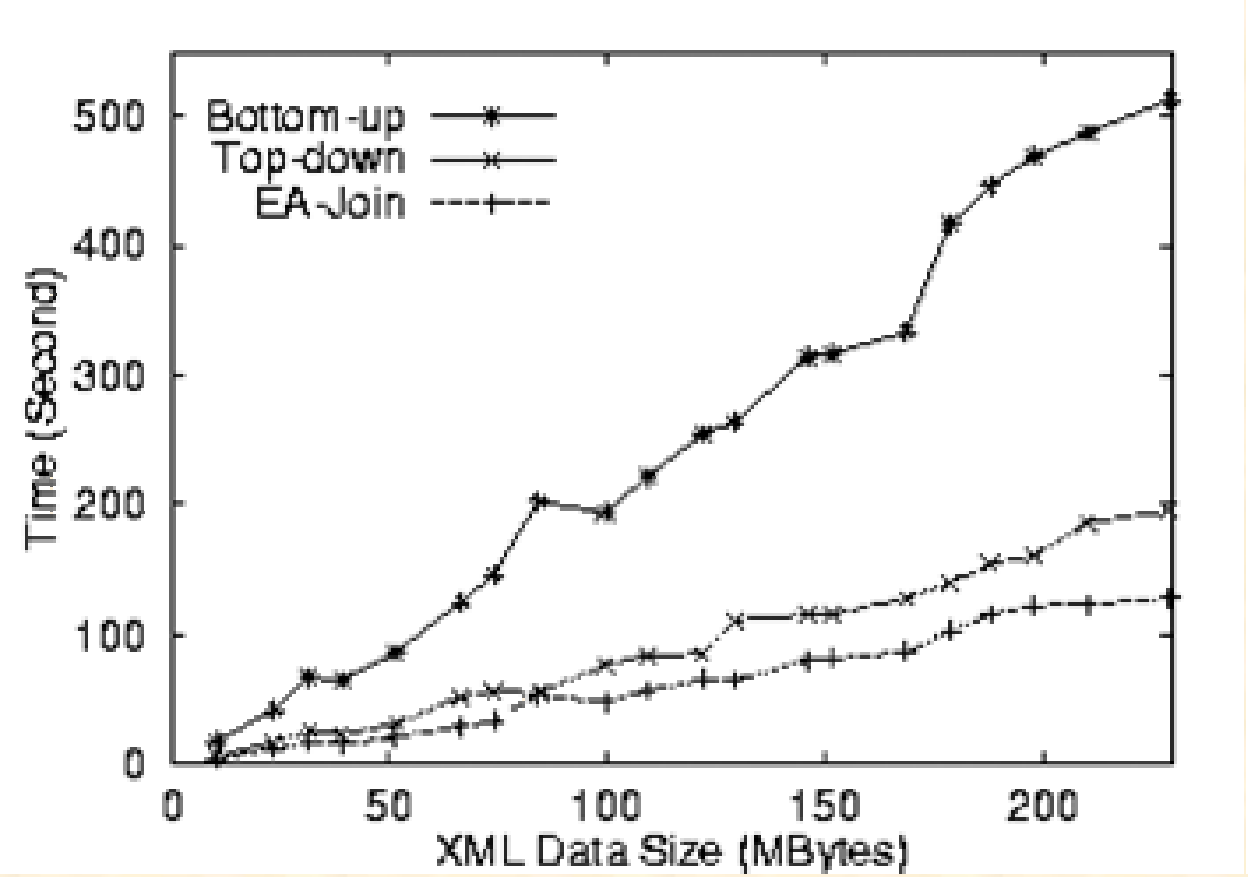


EA-Join: Speed-up



EA-Join: Scale-up

- **NITF data (229MB)**



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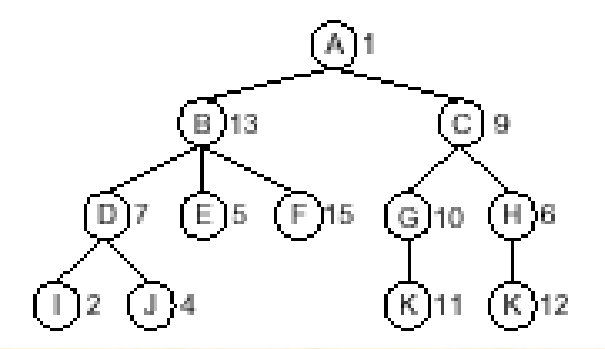
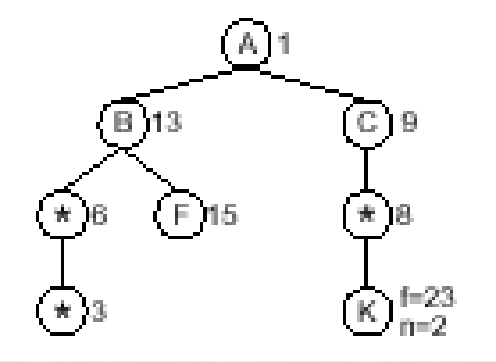
Selectivity Estimation

- **Path Tree [VLDB'01]**
  - **Path Tree is a condensed form of XML data tree**
    - **Each node labeled with a tag name and a frequency**
    - **Use *-nodes to coalesce nodes and frequencies**
  - **To estimate, take the frequency sum, or average if there is a *-node in the path.**



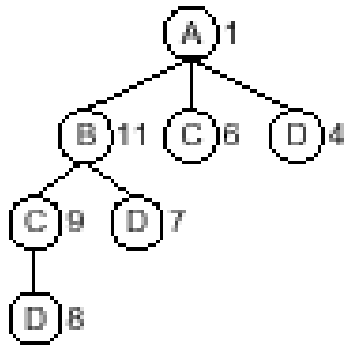
XML data tree



Path tree

Selectivity Estimation

- **Markov Table [VLDB'01]**
  - **Store frequencies of paths no longer than *M***
  - **Use *short memory* assumption to estimate frequencies for paths longer than *M***
    - **Freq(A/B/C/D) = freq(A/B/C)Pr(D | B/C)**
      = freq(A/B/C)freq(B/C/D)/freq(B/C)



Path	Freq	Path	Freq
A	1	AC	6
B	11	AD	4
C	15	BC	9
D	19	BD	7
AB	11	CD	8

$$freq(A/B/C) = freq(A/B)\frac{freq(B/C)}{freq(B)} = 9$$

$$freq(A/B/C/D) = freq(A/B)\frac{freq(B/C)}{freq(B)}\frac{freq(C/D)}{freq(C)} = 4.8$$

Selectivity Estimation

- **Positional Histogram [EDBT'02]**
  - Query: $u[P_1]//v[P_2]$
  - Associate an *extended preorder* with each node
    - Each node mapped into a point in a 2-dim space
    - Intervals either *separate* or *fully contained*
    - Ancestors in the upper-left region, and descendants in the lower-right region
  - To estimate the selectivity of $u[P_1]//v[P_2]$
    - Estimate the number of *ancestors (or descendants)* for each instance of *v (or u)* using the 2-dim histogram

Concluding Remarks

- **XML for a wide spectrum of applications**
  - **Bioinformatics, Multimedia (Mpeg), Chemistry**
  - **Literature, Patent/Financial/Legal, Metadata Exchange**
  - ***The list of applications keeps increasing!!***
  - **See *XML Cover Page* for more applications**
    - **CML (Chemical Markup Language)**
    - **HDML (Hand-held Device Markup Language)**
    - **WIDL (Web Interface Definition Language)**
- **XML poses new challenges**
  - **Relational vs. Semi-structured: Mapping required**
  - **Indexing and Querying XML data**
  - **XML query optimization and selectivity estimation**

Still Going On and On…

- ACM SIGMOD'2002
  - 10 out of 42 research papers related to XML data
    - Indexing for path queries, joins, storing in RDB, semi-structured, statistics, etc.
  - 1 industrial paper and 4 demos
- At the U of Arizona
  - Optimization of Path Joins with Long paths
  - Comparative performance study (e.g., Index Fabric)
  - Implementation of XISS and Path Joins on RDBMS
  - Launch the MDR (Microarray Data Repository) project in collaboration with researchers at AHSC

Questions

For more information,

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