Advanced databases and data models:

Theme3: Efficient storage of XML

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Today´s lecture

Native XML management
Shredding
Hybrid solutions
- SQL/XML
- HShreX
- Efficency

XML as a data model

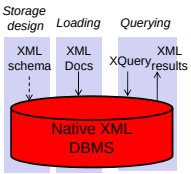
XML is richer than the relational model
- Tree structure,
- Order
- …

Vary from highly structured to unstructured
- Database export
- …
- Annotated text documents

Can contain links to other type of entities

What does this mean for efficient storage?

Storage possibilities for XML

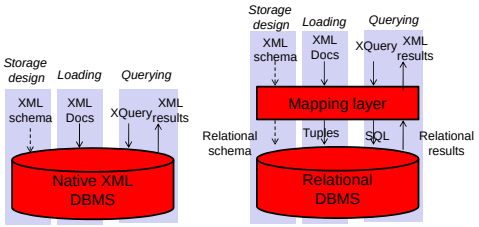


Native XML databases

- Defines a (logical) model for an XML document
  - Elements, attributes, PCDATA, document order.
- The XML document is the logical unit of storage
- Can have any physical underlying storage model
- Often: grouping documents, collections
- Query model: Xpath and in most cases Xquery

- Examples:
  - eXist http://exist-db.org/
  - MarkLogic http://www.marklogic.com

Storage possibilities for XML



Shredding

How to shred XML?

```
<families
xmlns:xsi=http://www.w3.org/2001/XMLSchem
a-instance>
  <family>
    <parent>
      <name>Lena</name>
      <job>Lektor</job>
    </parent>
    <child>
      <name>Ludvig</name>
      <school>Skolan</school>
    </child>
  </family>
</families>
```

Source	Ordinal	attrName	isValue	Value
0	1	Families	False	1
1	1	Family	False	2
2	1	Parent	False	3
3	1	Name	True	Lena
3	2	Job	True	Docent ..

Families

Id	Pid
0	-

Family

Id	Pid
1	0

Parent

Id	Pid	Name	Job
2	1	Lena	Lektor

Child

Id	Pid	Name	School
3	1	Ludvig	Skolan

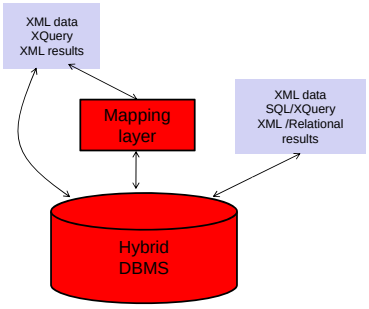
Related work

Shredding of XML into relational storage

Bohannon et al. 2002, (ICDE),
Florescu and Cossman 1999 (IEEE Data Eng),
Georgiadis and Vassalos 2007 (SIGMOD),

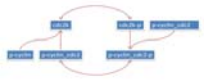
Grust et al. (2007) (SIMOD),
Mlynkova 2009 (DEXA)

Hybrid XML Storage



New possibilities…

```
<model id="Tyson1991CellModel_6"
       name="Tyson1991_CellCycle_6var">
 <listOfSpecies>
   + <species id="C2" name="cdc2k" compartment="cell">
   + <species id="M" name="p-cyclin_cdc2" compartment="cell">
   + <species id="YP" name="p-cyclin" compartment="cell"> ...
 </listOfSpecies>
 <listOfReactions>
  <reaction id="Reaction1" name="cyclin_cdc2k dissociation">
   <annotation>
     <rdf:li rdf:resource="http://www.reactome.org/#REACT_6308"/>
     <rdf:li rdf:resource="http://www.geneontology.org/#GO:0000079"/>
   </annotation>
   <listOfReactants>
     <speciesReference species="M"/>
   </listOfReactants>
   <listOfProducts>
     <speciesReference species="C2"/>
     <speciesReference species="YP"/>
   </listOfProducts>
   <kineticLaw>
     <math xmlns="http://www.w3.org/1998/Math/MathML">
       <apply> <times/> <ci> k6 </ci> <ci> M </ci>  </apply></math>
     <listOfParameters>   <parameter id="k6" value="1">
     </listOfParameters>
   </kineticLaw>
  </reaction>
  + <reaction id="Reaction2" name="cdc2k phosphorylation">
   ... more reactions
 </listOfReactions>
</model>
</sbml>
```



Species:

id	Name	Compartment
C2	cdc2k	cell
M	p-cyclin_cdc2	cell
YP	p-cyclin	cell
....	....	....

Reaction:

id	Name	Annotation	Formula
Reaction1	cyclin_cdc2k dissociation	<annotation ....>	<kinetic_law ....>
Reaction2	cdc2k phosphorylation	<annotation ....>	<kinetic_law ....>
....	....	....	....

Reactants:

id	Species
Reaction1	M
Reaction2	....
	....

Products:

id	Species
Reaction1	C2
Reaction1	YP
	....

Hybrid storage and SQL/XML

Hybrid XML storage
- Beyer et al.
- Hua Liu et al.
- Rys et al. (2005) (SIGMOD)

Proposed as SQL standard

Available in: DB2, Microsoft SQL Server, Oracle

More limited versions in other databases….

XML type

CREATE TABLE:

```
create table sbml_data (sbml_doc XML);

create table reaction (
    id varchar(100) not null,
    name varchar(250),
    math XML,
    annotation XML,
    primary key(id)
)
```

Querying

```
select
    sbml_doc.query('/sbml/model/listOfSpecies/species[@id
    = "C2"]')
from sbml_data;

<species id="C2" name="cdc2k" compartment="cell">
  <annotation> …</annotation>
</species>
```

Querying

```
select reactome_doc.query(
'for $react in /model/listOfReactions/reaction
return <path>
    <from> {data($react/listOfReactants/speciesReference/@species)}
    </from>
      <via> {data($react/@id)} </via>
    <to> {data($react/listOfProducts/speciesReference/@species)} </to>
</path>')
from reactome_data;

<path><from>M</from><via>Reaction1</via><to>C2</to></path>
<path><from>M</from><via>Reaction1</via><to>YP</to></path>
…
```

Transforming data to relations

```
insert into reaction(id, name, annotation, formula)
select   r.value('@id','varchar(100)') as id,
         r.value('@name','varchar(250)') as name,
         r.value('annotation','xml') as annotation,
         r.value('kinetic formula','xml') as formula,
from
  (select
      sbml_doc
    .nodes(sbml/model/listOfReactions/reaction‘)
  from sbml_data) as d(r);
```

Transforming data to XML

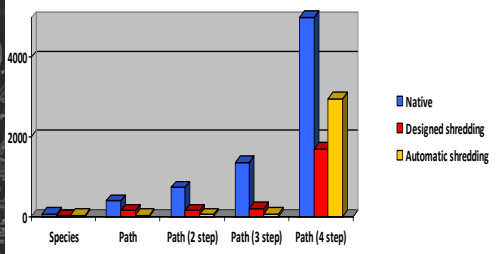
```
select reaction.reaction as name, reaction.id,
  (select
     (select speciesReference.reactant as species from reactants
    speciesReference where reaction.id = speciesReference.id
       for XML auto, type)
   from emptyXML as listOfReactants for XML auto, type),
  (select
     (select speciesReference.product as species from products
    speciesReference where reaction.id = speciesReference.id
       for XML auto, type)
   from emptyXML as listOfProducts for XML auto, type) ,
from reaction
for XML auto, type
```

Syntax differs between DBMS´s (DB2)

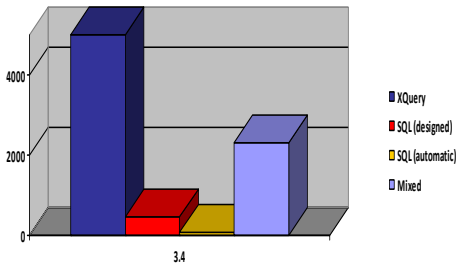
```
select  sbml_doc.query(
'for $y in /model/listOfReactions/reaction/listOfModifiers/modifierSpeciesReference,
    $z in /model/listOfSpecies/species[@id = $y/@species]
return <modifier> {$y/@species} {$y/../../@id} {$z/@compartment} </modifier>')
from reactome_data;

xquery
for
    $y in db2-fn:xmlcolumn('REACTOME_DATA.REACTOME_DOC')/model/
            listOfReactions/reaction /listOfModifiers/modifierSpeciesReference,
    $z in db2-fn:xmlcolumn('REACTOME_DATA.REACTOME_DOC')/model/
        listOfSpecies/species[@id = $y/@species]
return <modifier> {$y/@species} {$y/../../@id} {$z/@compartment} </modifier>
```

Efficiency: Increasing query complexity

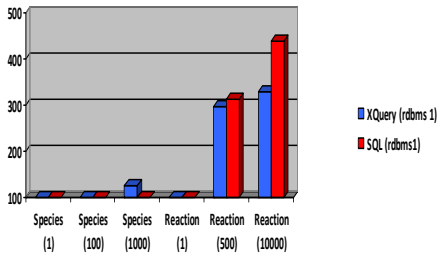


Efficiency: Combining representations



3.4

Efficiency: Return the result as XML



Higher complexity

Numerous alternatives for XML storage
How to achieve models that are efficient and easy to use
Dependent on application, XML data and query load

What are we doing?

Efficiency studies

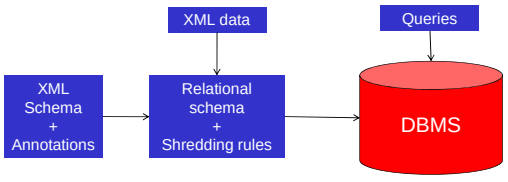
Guidelines

Tool development

Guidelines:

Keep together what naturally belong together
Do not shred parts of the XML where the schema allows large variation
Take variations of the actual data into account
Shred elements that are critical for performance
Prefer the representation that is required for query results
Avoid shredding where future versions of the schema is likely to change.
Avoid shredding if parallel versions of data is to be kept

HShreX – a tool for evaluation



Extension of an old tool Shrex to allow hybrid storage

Working with HShreX:

```
<?xml version="1.0" encoding="UTF-8"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema"
    xmlns:shrex="http://www.cse.ogi.edu/shrex">

  <xs:element name="families">
    <xs:complexType>
      <xs:sequence maxOccurs="unbounded">
        <xs:element name="family" type="familyType"/>
      </xs:sequence>
    </xs:complexType>
  </xs:element>

  <xs:complexType name="familyType">
    <xs:sequence>
      <xs:element name="parent" type="parentType" >
      <xs:element name="child" type="childType" >
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="parentType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="job" type="xs:string"/>
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="childType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="school" type="xs:string"/>
    </xs:sequence>
  </xs:complexType>
</xs:schema>
```

Families

Id	Pid
0	-

Families_family

Id	Pid
1	0

Families_family_parent

Id	Pid	Name	Job
2	1	Lena	Lektor

Families_family_child

Id	Pid	Name	School
3	1	Ludvig	Skolan

Working with HShreX:

```
<?xml version="1.0" encoding="UTF-8"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema"
    xmlns:shrex="http://www.cse.ogi.edu/shrex">

  <xs:element name="families">
    <xs:complexType>
      <xs:sequence maxOccurs="unbounded">
        <xs:element name="family" type="familyType"/>
      </xs:sequence>
    </xs:complexType>
  </xs:element>

  <xs:complexType name="familyType">
    <xs:sequence>
      <xs:element name="parent" type="parentType" >
      <xs:element name="child" type="childType"
                  shrex:maptoxml="true" >
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="parentType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="job" type="xs:string"/>
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="childType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="school" type="xs:string"/>
    </xs:sequence>
```

Families

Id	Pid
0	-

Families_family

Id	Pid	Child
1	0	<child> <name>Ludvig</name> <school>Skolan/school> </child>

Families_family_parent

Id	Pid	Name	Job
2	1	Lena	Lektor

Working with HShreX:

```
<?xml version="1.0" encoding="UTF-8"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema"
    xmlns:shrex="http://www.cse.ogi.edu/shrex">

  <xs:element name="families">
    <xs:complexType>
      <xs:sequence maxOccurs="unbounded">
        <xs:element name="family" type="familyType"/>
      </xs:sequence>
    </xs:complexType>
  </xs:element>

  <xs:complexType name="familyType">
    <xs:sequence>
      <xs:element name="parent" type="parentType"
                  shrex:tablename="person">
      <xs:element name="child" type="childType"
                  shrex:tablename="person" >
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="parentType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="job" type="xs:string"/>
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="childType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="school" type="xs:string"/>
```

Families

Id	Pid
0	-

Families_family

Id	Pid
1	0

Person

Id	Pid	Name	Job	School
2	1	Lena	Lektor	
3	1	Ludvig		Skolan

Working with HShreX:

```
<?xml version="1.0" encoding="UTF-8"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema"
    xmlns:shrex="http://www.cse.ogi.edu/shrex">

  <xs:element name="families">
    <xs:complexType>
      <xs:sequence maxOccurs="unbounded">
        <xs:element name="family" type="familyType"/>
      </xs:sequence>
    </xs:complexType>
  </xs:element>

  <xs:complexType name="familyType">
    <xs:sequence>
      <xs:element name="parent" type="parentType"
                  shrex:withparenttable="true">
      <xs:element name="child" type="childType" >
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="parentType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="job" type="xs:string"/>
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="childType">
    <xs:sequence>
      <xs:element name="name" type="xs:string"/>
      <xs:element name="school" type="xs:string"/>
    </xs:sequence>
```

Families

Id	Pid
0	-

Families_family

Id	Pid	Name	Job
1	0	Lena	Lektor

Families_family_child

Id	Pid	Name	School
3	1	Ludvig	Skolan

HShrex Demo

Use case: Modelling

	Data model	Native	Mixed	Shredded
SBML	*Nr of annotations*	1	21	0
	Nr of relations	3	8	121
UniProt	*Nr of annotations*	1	24	0
	Nr of relations	2	32	121

Annotations

maptoxml
ignore
withparenttable
outline
tablename
fieldname
sqltype

Use case: Querying

Mixed

```
select m.species
from reaction r, modifier m
where r.shrex_id = m.shrex_pid and
r.name=react1;
```

Shredded

```
select  m.species
from sbml_model_listOfReactions_reaction r,
sbml_model_listOfReactions_reaction_l
istOfModifiers_modifiersSpeciesReference p,
sbml_model_listOfReactions_reaction_l
istOfModifiers lm
where m.shrex_pid = lm.shrex_id and
   lm.shrex_pid = r.shrex_id and
   r.name = React1';
```

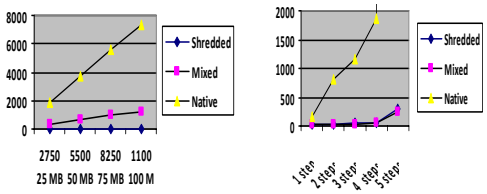
Native:

```
select entry.query('data(//uniprot:accession)')
from uniprot_entry
where entry.exist(//uniprot:subcellularLocation
        [uniprot:location/text()="Cytoplasm"])=1;
```

Mixed:

```
select accession
from uniprot_entry_accession, entry,
uniprot_entry_comment
where
comment.exist(//uniprot:subcellularLocation[uni
prot:location/text()= "Cytoplasm"])=1
and uniprot_entry_comment.shrex_pid =
entry.shrex_id
and uniprot_entry_accession.shrex_pid =
entry.shrex_id
```

Use case: Efficiency



Lab exercises

Use HShreX for performance studies.

Three suggested datasets:
- SBML (Reactome)
- SBML (Biomodels)
- PSI MI
- Michigan Benchmark

If own data – check with the lab assistant

For + select own of several tasks

NoSQL – non relational databases

Examples:
Document store: CouchDB, ApacheDB
XML database: Marklogic Server, eXist
Graph: AllegroGraph, Neo4j
Object database: GemStone/S
Key/value store on disk: BigTable
Eventually consistent key-value store: Cassandra
Ordered Key-value store: Berkeley DB
Tabular: BigTable, HyperTable, Hbase
Tuple store: Apache River

Neo

Neo4j is a **graph database**. It is an embedded, disk-based, fully transactional Java persistence engine that stores data structured in graphs rather than in tables.

Linköping related company.

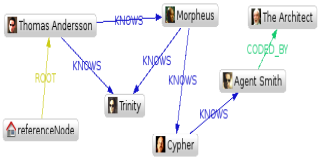
Interesting for semi-structured data.

The Neo Persistence Engine

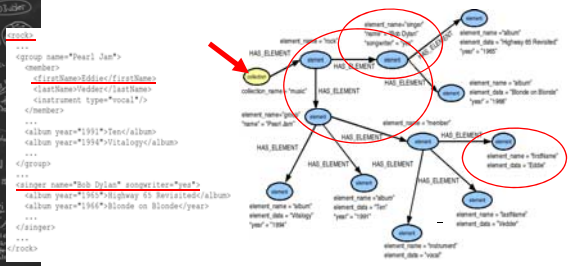
Primitives:
- nodes,
- relationships
- properties

Features
- ACID transaction
- Durable persistence
- Transaction recovery

Implementation
- Java



Representing XML in Neo: Basic solution



Representing XML in Neo: Customizations

Yahoo!: A web of concepts

- Concept: Things of interest to the users of the web.
- Concept represented as:
  - Id
  - meta-data (attributes with values)
- Goals: Concept centric data organization
- What to support:
  - Nested structure?
  - Provenance, versions uncertainty?
  - Relations between concepts?

What do we search for?

Individual concepts: 60-70% Sets of concepts 10-20%

Attributes of a concept:
Rather small correlation (restaurant menu 3%)

Aggreation: 59% of users click on more than one URL.

Concepts vs. Browsing: Follow paths of how user browsed.
Easy to find patterns of what users commonly visit.