XML and Databases

Chapter 7: XML Schema III: Keys and Derived Types

Prof. Dr. Stefan Brass

Martin-Luther-Universität Halle-Wittenberg

Winter 2022/23

http://www.informatik.uni-halle.de/~brass/xml22/

Objectives

After completing this chapter, you should be able to:

- use keys and key references in an XML Schema.
- compare keys in XML Schema with keys in the relational model.
- declare derived complex types in XML schema.
- compare type derivation in XML schema with subclasses in XML schema.
- respect the possible existence of derived types when developing programs to process XML data.

Contents

Integrity Constraints (1)

- DTDs have `ID`/`IDREF` to permit a unique identification of nodes and links between elements.
- This mechanism is quite restricted:
  - The identification must be a single XML name.

    A number cannot be used as identification. Composed keys are not supported. DTDs do not allow further restrictions of the possible values, e.g. one cannot enforce a certain format for the names.
  - The scope is global for the entire document.

    One cannot state that the uniqueness only has to hold within an element (e.g., representing a relation). One cannot specify any constraints of the element type that is referenced with `IDREF`.
  - This works only for attributes, not for elements.

Integrity Constraints (2)

- XML Schema has mechanisms corresponding to keys and foreign keys in relational databases that solve the problems of `ID`/`IDREF`.

  They are more complex than the relational counterparts, because the hierarchical structure of XML is more complex than the flat tables of the relational model. The simplicity of the relational model was one of its big achievements. This is given up in XML databases.

- The facets correspond to `CHECK`-constraints that restrict the value set of a single column.

  Not all SQL conditions that refer to only one column can be expressed with facets. On the other hand, patterns in XML Schema are much more powerful than SQL's `LIKE`-conditions. It is strange that patterns refer to the external representation.

Integrity Constraints (3)

- Otherwise, XML Schema 1.0 is not very powerful with respect to constraints. This changed in Version 1.1.

  E.g., `CHECK`-constraints in relational databases can state logical conditions between the column values of a table row, e.g. if one column has a certain value then another column must be not null. The facets of XML Schema constrain only single values.

- For example, XML Schema itself requires that the `type`-attribute of `element` is mutually exclusive with `simpleType`/`complexType`-child elements.

- This constraint cannot be specified in XML Schema 1.0.

  One would expect that the schema for XML Schema can express the necessary requirements.

Integrity Constraints (4)

- XML Schema 1.1 (released April 5, 2012) introduced an Element `assert` that permits to specify arbitrary conditions in XPath 2.0.

  However, there are not very many XML Schema 1.1 implementations yet.

- For instance, one can compare two attribute values of an element (attribute `min` must be $\leq$ `max`):

```
<xs:complexType name="intRange">
    <xs:attribute name="min" type="xs:int"/>
    <xs:attribute name="max" type="xs:int"/>
    <xs:assert test="@min le @max"/>
</xs:complexType>
```

[https://www.w3.org/TR/2012/REC-xmlschema11-1-20120405/]

Contents

Unique/Key Constraints (1)

- Consider again the example:

```
<?xml version='1.0' encoding='ISO-8859-1'?>
<GRADES-DB>
  <STUDENTS>
    <STUDENT>
      <SID>101</SID>
      <FIRST>Ann</FIRST>
      <LAST>Smith</LAST>
    </STUDENT>
    ...
  </STUDENTS>
  ...
</GRADES-DB>
```

Unique/Key Constraints (2)

- SID-values uniquely identify the children of STUDENTS:

```
<xs:element name="STUDENTS">
  <xs:complexType>
    <xs:sequence>
      <xs:element ref="STUDENT"
          minOccurs="0" maxOccurs="unbounded"/>
    </xs:sequence>
  </xs:complexType>
  <xs:unique name="STUDENTS_KEY">
    <xs:selector xpath="*"/>
    <xs:field xpath="SID"/>
  </xs:unique>
</xs:element>
```

Unique/Key Constraints (3)

- There are three components to a `unique`-constraint (basically corresponds to relation, row, column(s)):
  - The scope, which delimits the part of the XML document, in which the uniqueness must hold.

    Every element of the type in which the `unique`-constraint is defined is one such scope.
  - The elements which are identified.

    The XPath-expression in `selector` specifies how to get from a scope-element to these elements ("target node set").
  - The values which identify these elements.

    The XPath-expressions in one or more `field`-elements specify how to get from the identified elements to the identifying values.

Unique/Key Constraints (4)

- In the example:
  - The scope is the STUDENTS-element.

    In the example, there is only one STUDENTS-element. If there were more than one, the uniqueness has to hold only within each single element.
  - The elements that are identified are the children of STUDENTS (the STUDENT-elements).

    One could also write `xpath="STUDENT"`.
  - The value that identifies the elements is the value of the SID-child.

Unique/Key Constraints (5)

- The correspondence of the scope to a relation is not exact:
  - In the example, it is also possible to define the entire document as scope, but to select only `STUDENT`-elements (see next slide).
  - In contrast to the `ID`-type, it is no problem if other keys contain the same values.

    Even if the scope is global, the uniqueness of values must hold only within a key (i.e. one could say that the scope is the key).
- Only values of simple types can be used for unique identification.

Unique/Key Constraints (6)

- SID-values uniquely identify STUDENT-elements:

```
<xs:element name="GRADES-DB">
  <xs:complexType>
    <xs:sequence>
      <xs:element ref="STUDENTS"/>
      <xs:element ref="EXERCISES"/>
      <xs:element ref="RESULTS"/>
    </xs:sequence>
  </xs:complexType>
  <xs:unique name="STUDENTS_KEY">
    <xs:selector xpath="STUDENTS/STUDENT"/>
    <xs:field xpath="SID"/>
  </xs:unique>
</xs:element>
```

Unique/Key Constraints (7)

- Example with composed key:

```
<xs:element name="GRADES-DB">
  <xs:complexType>
    <xs:sequence>
      <xs:element ref="STUDENTS"/>
      <xs:element ref="EXERCISES"/>
      <xs:element ref="RESULTS"/>
    </xs:sequence>
  </xs:complexType>
  <xs:unique name="EXERCISES_KEY">
    <xs:selector xpath="EXERCISES/*"/>
    <xs:field xpath="CAT"/>
    <xs:field xpath="ENO"/>
  </xs:unique>
</xs:element>
```

Unique/Key Constraints (8)

- Suppose we store the data in attributes:

```
<EXERCISE CAT='H' ENO='1'
    TOPIC='Rel. Algeb.' MAXPT='10'/>
```

- Attributes as fields are marked with "@":

```
<xs:element name="GRADES-DB">
  ...
  <xs:unique name="EXERCISES_KEY">
    <xs:selector xpath="EXERCISES/*"/>
    <xs:field xpath="@CAT"/>
    <xs:field xpath="@ENO"/>
  </xs:unique>
</xs:element>
```

Unique/Key Constraints (9)

- Example with exercise info nested in categories:

```
<EXERCISES>
  <CATEGORY CAT="H">
    <EX ENO="1" TOPIC="Rel. Algeb." MAXPT="10"/>
    <EX ENO="2" TOPIC="SQL" MAXPT="10"/>
  </CATEGORY>
  <CATEGORY CAT="M">
    <EX ENO="1" TOPIC="SQL" MAXPT="14"/>
  </CATEGORY>
</EXERCISES>
```

- XML Schema supports only a subset of XPath.
  In particular, one cannot access ancestors in `xs:field`.
  But the unique identification of `EX` needs `CAT`.

Unique/Key Constraints (10)

- The problem is solved by defining two keys:
  - One key ensures that the CAT-value uniquely identifies CATEGORY-elements.
  - The other key is defined within the CATEGORY element type (thus, there is one instance of the key, i.e. scope, for every category element). This key ensures the unique identification of EX-elements by the ENO within each CATEGORY element.
- However, in this way no foreign keys can be specified that reference EX-elements by CAT and ENO.

Unique/Key Constraints (11)

- Key on CATEGORY:

```
<xs:element name="GRADES-DB">
  ...
  <xs:unique name="CATEGORY_KEY">
    <xs:selector xpath="EXERCISES/CATEGORY"/>
    <xs:field xpath="@CAT"/>
  </xs:unique>
</xs:element>
```

The XPath-expression in `selector` could also be `EXERCISES/*` (because `EXERCISES` has only `CATEGORY`-elements as children).
One could define the key also under `EXERCISES` (instead of `GRADES-DB`) since the document contains only one element of type `EXERCISES`, and all elements to be identified are nested within this element.

Unique/Key Constraints (12)

- Key on EX-elements within CATEGORY:

```
<xs:element name="CATEGORY">
  ...
  <xs:unique name="EX_KEY">
    <xs:selector xpath="*"/>
    <xs:field xpath="@ENO"/>
  </xs:unique>
</xs:element>
```

- It is no problem that there are two EX-elements with the same ENO (e.g., 1) as long as they are nested within different CATEGORY-elements.
- This is similar to a weak entity.

Unique/Key Constraints (13)

- For a given "context node" (in which the key is defined), the selector defines a "target node set".
- For each node in the target node set, the XPath-expression in each field must return 0 or 1 values. It is an error if more than one value is returned.
- The target nodes, for which each field has a value (that is not nil), form the "qualified node set".
- The unique identification is required only for the qualified node set. Multiple elements with undefined or partially defined key values can exist.

Unique/Key Constraints (14)

- If one writes `xs:key` instead of `xs:unique`, the fields must exist.
  - In this case, it is an error if the XPath-expression in `xs:field` returns no values.
  - And it is always an error if it returns more than one value.

    Furthermore, neither the identified nodes nor the identifying fields may be nillable.
- Note that value equality respects the type:
  - For a field of type `integer`, `"03"` and `"3"` are the same (so the uniqueness would be violated).
  - For a field of type `string`, they are different.

Contents

Key References (1)

- A "key reference" identity constraint corresponds to a foreign key in relational databases.
- It demands that certain (tuples of) values must appear as identifying values in a key constraint.

  "Key constraint" means `key` or `unique`.

- Example: For each `SID`-value in a `RESULT` element, there must be a `STUDENT`-element with the same `SID` (one can store points only for known students).

  As in relational databases, it is not required that the two fields have the same name.

Key References (2)

- SID-values in RESULT reference SID-values in STUDENT:

```
<xs:element name="GRADES-DB">

  ...

  <xs:key name="STUDENT_KEY">
    <xs:selector xpath="STUDENTS/STUDENT"/>
    <xs:field xpath="SID"/>
  </xs:key>

  <xs:keyref name="RESULT_REF_STUDENT"
      refer="STUDENT_KEY">
    <xs:selector xpath="RESULTS/RESULT"/>
    <xs:field xpath="SID"/>
  </xs:keyref>

</xs:element>
```

Key References (3)

- The referenced key must be defined in the same node or in a descendant node (i.e. “below”) the node in which the foreign key constraint is defined.

  I would have required the opposite direction, because on the way up, there could be only one instance of the referenced key, on the way down, there can be several (see below). But the committee certainly had reasons, probably related to the parsing/checking algorithms.

- The standard explains that “node tables” which map key values to the identified nodes are computed bottom-up.

  The standard talks of “key sequence” instead of “key values” to include also composed keys (with more than one field).

Key References (4)

- It is possible that several instances of the referenced key exist below the foreign key.
- In that case, the union of the node tables is taken, with conflicting entries removed.

  I.e. if two instances of the referenced key contain the same key value with different identified nodes, that key value is removed from the table: It cannot be referenced (the reference would not be unique).
  The situation is even more complicated, if the key is defined in an element type that has descendants of the same type. Then key value-node pairs originating in the current node take precedence over pairs that come from below. Values that come from below are only entered in the node table if they do not cause a conflict.

Key References (5)

- Fields of key and foreign key are matched by position in the identity constraint definition, not by name (as in relational databases).
- Normally, the types of corresponding fields (of the key and the foreign key) should be the same.
- However, if the types of both columns are derived from the same primitive type, it might still work (for values in the intersection of both types).
- But values of unrelated types are never identical: E.g. the string "1" is different from the number "1".

Contents

Derived Complex Types (1)

- There are two ways to derive complex types:
  - by extension, e.g. adding new elements at the end of the content model, or adding attributes,
  - by restriction, e.g. removing optional elements or attributes, or restricting the data type of attributes, etc.
- Derived simple types are always restrictions.

  One can extend a simple type by adding attributes, but then it becomes a complex type.

Derived Complex Types (2)

- Extension looks very similar to subclass definitions in object-oriented languages.

  There all attributes from the superclass are inherited to the subclass, and additional attributes can be added.

- However, a basic principle in object-oriented languages is that a value of a subclass can be used wherever a value of the superclass is needed.

- In XML, it depends on the application, whether it breaks if there are additional elements/attributes.

  Since XML Schema has this feature, future applications should be developed in a way that tolerates possible extensions.

Derived Complex Types (3)

- Additional attributes are probably seldom a problem, since attributes are typically accessed by name (not in a loop).
- It was tried to minimize the problems of additional child elements by allowing them only at the end of the content model.
- Formally, the content model of the extended type is always a `sequence` consisting of
  - the content model of the base type,
  - the added content model (new child elements).

Derived Complex Types (4)

- Consider a type for STUDENT-elements:

```
<xs:complexType name="STUDENT_TYPE">
  <xs:sequence>
    <xs:element name="SID"   type="SID_TYPE"/>
    <xs:element name="FIRST" type="xs:string"/>
    <xs:element name="LAST"  type="xs:string"/>
    <xs:element name="EMAIL" type="xs:string"
        minOccurs="0"/>
  </xs:sequence>
</xs:complexType>
```

- Suppose that exchange students must in addition contain the name of the partner university.

Derived Complex Types (5)

- Example for type extension:

```
<xs:complexType name="EXCHANGE_STUDENT_TYPE">
  <xs:complexContent>
    <xs:extension base="STUDENT_TYPE">
      <xs:sequence>
        <xs:element name="PARTNER_UNIV"
            type="UNIV_TYPE"/>
      </xs:sequence>
    </xs:extension>
  </xs:complexContent>
</xs:complexType>
```

- The effective content model is now:

```
((SID, FIRST, LAST, EMAIL?), (PARTNER_UNIV))
```

Derived Complex Types (6)

- In the same way, one can add attributes. Suppose that STUDENT_TYPE2 has attributes SID, FIRST, LAST, EMAIL (and empty content).
- Then a new attribute is added as follows:

```
<xs:complexType name="EXCHANGE_STUDENT_TYPE2">
  <xs:complexContent>
    <xs:extension base="STUDENT_TYPE2">
      <xs:attribute name="PARTNER_UNIV"
          type="UNIV_TYPE" use="required"/>
    </xs:extension>
  </xs:complexContent>
</xs:complexType>
```

Derived Complex Types (7)

- Let us return to the case where STUDENT has child elements SID, FIRST, LAST, EMAIL.
- The type of EMAIL might be a simple type:

```
<xs:simpleType name="EMAIL_TYPE">
  <xs:restriction base="xs:string">
    <xs:maxLength value="80"/>
  </xs:restriction>
</xs:simpleType>
```

- Suppose that an attribute must be added that indicates whether emails can be formatted in HTML or must be plain text.

Derived Complex Types (8)

- When an attribute is added to a simple type, one gets a complex type:

```
<xs:complexType name="EMAIL_TYPE2">
  <xs:simpleContent>
    <xs:extension base="EMAIL_TYPE">
      <xs:attribute name="HTML_OK"
          type="xs:boolean" use="optional"/>
    </xs:extension>
  </xs:simpleContent>
</xs:complexType>
```

- Example (element `EMAIL` of type `EMAIL_TYPE2`):

```
<EMAIL HTML_OK="false">brass@acm.org</EMAIL>
```

Derived Complex Types (9)

- If one uses restriction to define a derived type, it is guaranteed that every value of the derived type is also a valid value of the original type.
- If one wants to restrict a content model, one must repeat the complete content model.

  I.e. also the unmodified parts must be listed. The restricted content model does not have to be structurally identical. E.g. groups with only a single element can be eliminated (if `minOccurs` and `maxOccurs` are both 1), a `sequence` group with `minOccurs="1"` and `maxOccurs="1"` can be merged with an enclosing `sequence` group, the same for `choice`-groups. However, for `all` and `choice` groups, subgroups must be listed in the same order, although the sequence is semantically not important.

Derived Complex Types (10)

- If one wants to restrict an attribute, it suffices to repeat only this attribute.
- Consider again STUDENT_TYPE2 with attributes SID, FIRST, LAST, EMAIL. The optional attribute EMAIL can be removed as follows:

```
<xs:complexType name="STUDENT_TYPE3">
  <xs:complexContent>
    <xs:restriction base="STUDENT_TYPE2">
      <xs:attribute name="EMAIL"
          use="prohibited"/>
    </xs:restriction>
  </xs:complexContent>
</xs:complexType>
```

Derived Complex Types (11)

- The same change for the type STUDENT with child elements SID, FIRST, LAST, EMAIL (minOccurs="0"):

```
<xs:complexType name="STUDENT_TYPE4">
 <xs:complexContent>
  <xs:restriction base="STUDENT_TYPE">
    <xs:sequence>
      <xs:element name="SID"   type="SID_TYPE"/>
      <xs:element name="FIRST" type="xs:string"/>
      <xs:element name="LAST"  type="xs:string"/>
    </xs:sequence>
  </xs:restriction>
 </xs:complexContent>
</xs:complexType>
```

Derived Complex Types (12)

- Possible restrictions for complex types:
  - Optional attribute becomes required/prohibited.
  - The cardinality of elements or model groups becomes more restricted (`minOccurs` ↑, `maxOccurs` ↓).
  - Alternatives in `choice`-groups are reduced.
  - A restricted type can be chosen for an attribute or a child element.
  - A default value can be changed.
  - An attribute or element can get a fixed value.
  - Mixed content can be forbidden.

Contents

Documentation, App. Info (1)

- Documentation about the schema can be stored within the XML Schema definition.

  And not only as XML comments: Many XML tools suppress comments, and very little formatting can be done there.

- This is one purpose of the `annotation` element type, which is allowed
  - as first child of every XML Schema element type

    But it cannot be nested, i.e. it cannot be used within `annotation` or its children `documentation` and `appinfo`.

  - anywhere as child of `schema` and `redefine`.

    There, multiple `annotation` elements are allowed. Inside all other element types, only one `annotation` element is permitted.

Documentation, App. Info (2)

- Many relational databases also have the possibility to store comments about tables and columns in the data dictionary.

  Of course, this is usually pure text, quite short and without formatting.

- The other purpose of the annotation element is to store information for tools (programs) that process XML Schema information within the schema.

  E.g. tools that compute a relational schema from an XML schema, and map data between the two, or tools that generate form-based data entry programs out of the schema data.

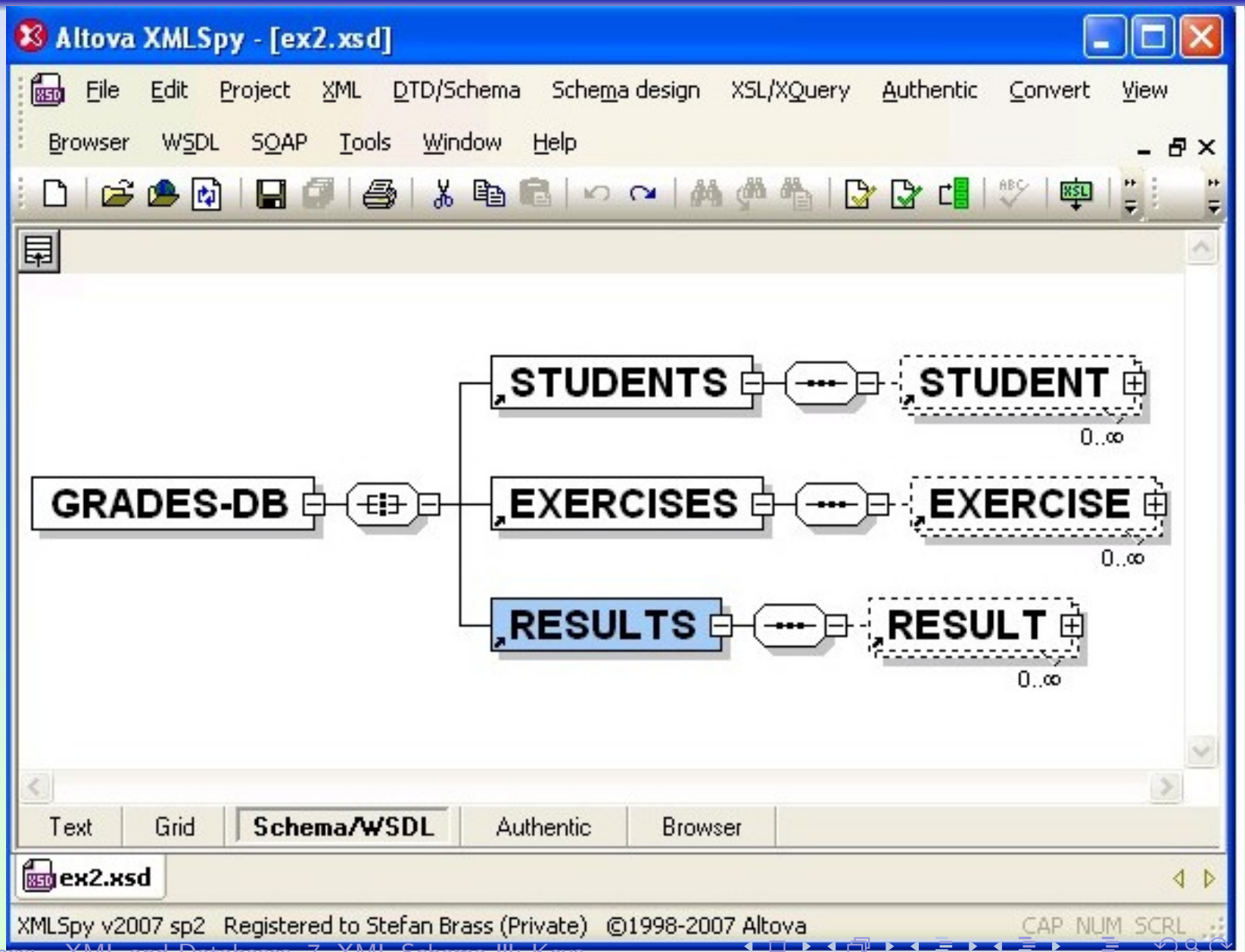
- This makes XML Schema extensible.

Documentation, App. Info (3)

- Example:

```
<xs:schema
    xmlns:xs="http://www.w3.org/2001/XMLSchema"
    xmlns:doc="http://doc.org/d1"
    xmlns:xsi=
        "http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation=
        "http://doc.org/d1 doc.xsd">
  <xs:element name="GRADES-DB">
    <xs:annotation>
      <xs:documentation xml:lang="en">
        <doc:title>Grades Database</doc:title>
        This is the root element.
        ...
    <xs:complexType>
        ...
```

Visualization of Schema Structure



References

- Harald Schöning, Walter Waterfeld: XML Schema.
  In: Erhard Rahm, Gottfried Vossen: Web & Datenbanken, Seiten 33-64.
  dpunkt.verlag, 2003, ISBN 3-89864-189-9.
- Priscilla Walmsley: Definitive XML Schema.
  Prentice Hall, 2001, ISBN 0130655678, 560 pages.
- W3C Architecture Domain: XML Schema.
  [http://www.w3.org/XML/Schema]
- David C. Fallside, Priscilla Walmsley: XML Schema Part 0: Primer.
  W3C, 28. October 2004, Second Edition.
  [http://www.w3.org/TR/xmlschema-0/]
- Henry S. Thompson, David Beech, Murray Maloney, Noah Mendelsohn:
  XML Schema Part 1: Structures.
  W3C, 28. October 2004, Second Edition
  [http://www.w3.org/TR/xmlschema-1/]
- Paul V. Biron, Ashok Malhotra: XML Schema Part 2: Datatypes.
  W3C, 28. October 2004, Second Edition
  [http://www.w3.org/TR/xmlschema-2/]
- [http://www.w3schools.com/schema/]