Annotated function3d XML schema (file function3d.xsd)

Version 2020-07-24

The quantum-simulation.org `function3d` XML Schema defines the allowed content of `function3d` documents according to the http://www.quantum-simulation.org specification. Validating XML parsers (such as Apache Xerces-C) use the XML Schema file "`function3d.xsd`" to verify the correctness of `function3d` documents.

XML header

```
<?xml version="1.0"?>
<schema xmlns="http://www.w3.org/2001/XMLSchema"
  targetNamespace="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0"
  xmlns:fpmd="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0">

  <annotation>
    <documentation>
      function3d.xsd, v1.0 (2020-07-24)
      http://www.quantum-simulation.org
      function3d XML Schema specification.
    </documentation>
  </annotation>
```

The header section contains the XML declaration of the `<schema>` element and the definition of the `XMLSchema` and `fpmd` namespaces. The `<annotation>` section describes the version of the `function3d` Schema specification. The current version is `2020-07-24` .

```
  <element name="function3d" type="fpmd:function3dType"/>
```

The body of the XML document consists of one element of type `function3dType`.

function3dType definition

```
  <complexType name="function3dType">
    <sequence minOccurs="0">
      <element name="domain" type="fpmd:domainType"/>
      <element name="reference_domain" minOccurs="0" type="fpmd:domainType"/
>
      <element name="grid" type="fpmd:gridType"/>
      <element name="grid_function" type="fpmd:grid_functionType"/>
    </sequence>
    <attribute name="name" type="fpmd:functionNameType" use="optional"/>
  </complexType>
```

The type `function3dType` element defines the components of a `function3d` element. It consists of a `<domain>` element, an optional `<reference_domain>` element, a `<grid>` element, a `<grid_function>` element and an optional `name` attribute. The `<domain>` and `<reference_domain>` element are used to represent unit cells in periodic lattices. The reference unit cell must enclose the unit cell. It is used in calculations involving variable unit cells.

domainType definition

```
  <complexType name="domainType">
```

```
    <attribute name="a" type="fpmd:d3vectorType" use="required"/>
    <attribute name="b" type="fpmd:d3vectorType" use="required"/>
    <attribute name="c" type="fpmd:d3vectorType" use="required"/>
  </complexType>
```

The type `domainType` defines a domain in 3-dimensional space and consists of three 3-vectors representing the lattice basis vectors. The unit cell and the reference unit cell are examples of elements of type domainType.

gridType definition

```
  <complexType name="gridType">
    <attribute name="nx" type="positiveInteger" use="required"/>
    <attribute name="ny" type="positiveInteger" use="required"/>
    <attribute name="nz" type="positiveInteger" use="required"/>
  </complexType>
```

The type `gridType` defines the size of the three-dimensional grid covering the domain.

gridfunctionType definition

```
  <complexType name="grid_functionType">
    <simpleContent>
      <extension base="string">
      <attribute name="type" type="fpmd:numericType" use="required"/>
      <attribute name="nx" type="positiveInteger" use="required"/>
      <attribute name="ny" type="positiveInteger" use="required"/>
      <attribute name="nz" type="positiveInteger" use="required"/>
      <attribute name="x0" type="nonNegativeInteger" default="0"/>
      <attribute name="y0" type="nonNegativeInteger" default="0"/>
      <attribute name="z0" type="nonNegativeInteger" default="0"/>
      <attribute name="encoding" type="fpmd:encodingType" use="required"/>
      <attribute name="href" type="anyURI" use="optional"/>
      </extension>
    </simpleContent>
  </complexType>
```

The type `grid_functionType` defines the values of the function on a subset of the grid defined in the `<grid>` element. The numeric type (double or complex) is specified by the `type` attribute. The nx, ny, nz, x0, y0, z0 attributes define the subset of the grid on which the function is defined. The subset of the grid has its origin at position (x0,y0,z0) in the grid, and has a size (nx,ny,nz). The encoding attribute (`text` or `base64`) is required to specify the type of encoding used for the data. The body of the `<grid_function>` element consists of a string that contains either a list of formatted values (if encoding=”`text`”) or base64-encoded data (if encoding=”`base64`”). The order of the elements corresponds to the following loop order:

```
for ( int k = 0; k < nz; k++ )
  for ( int j = 0; j < ny; j++ )
    for ( int i = 0; i < nx; i++ )
      write(f(i,j,k));
```

The `base64` encoded data must be consistent with a little-endian byte ordering. It is the responsibility of the application to convert the data on a big-endian architecture. This constraint ensures portability of function3d documents across architectures of varying byte-ordering. The optional `href` attribute can be used to point to the contents of another document.

Types used in the above definitions

```
  <simpleType name="d3vectorType">
    <restriction>
       <simpleType>
         <list itemType="double"/>
       </simpleType>
       <length value="3"/>
    </restriction>
  </simpleType>
```

The type `d3vectorType` defines a 3-vector. It consists of a list of three floating point numbers of type `double`.

```
  <simpleType name="numericType">
    <restriction base="string">
    <enumeration value="double"/>
    <enumeration value="complex"/>
    </restriction>
  </simpleType>
```

The type `numericType` defines the kind of function (double or complex) being represented.

```
  <simpleType name="encodingType">
    <restriction base="string">
    <enumeration value="text"/>
    <enumeration value="base64"/>
    </restriction>
  </simpleType>
```

The type `encodingType` defines the type of encoding (`text` or `base64`) used to represent function values as a string of characters.

```
  <simpleType name="functionNameType">
    <restriction base="string">
    </restriction>
  </simpleType>
```

The type `functionNameType` defines the type of the `name` attribute of the `function3d` element.

Example of function3d document

```
<?xml version="1.0" encoding="UTF-8"?>
<fpmd:function3d xmlns:fpmd="http://www.quantum-simulation.org/ns/fpmd/fpmd-
1.0"
 xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
 xsi:schemaLocation="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0
function3d.xsd"
 name="delta_v">
<domain a="16.0 0.0 0.0"
        b="0.0 16.0 0.0"
        c="0.0 0.0 16.0"/>
<grid nx="64" ny="64" nz="64"/>
<grid_function type="double" nx="64" ny="64" nz="64" encoding="base64">
```

```
AAAAAAAAAAAAAAAAAACgPwAAAAAAAMA/AAAAAAAA0j8AAAAAAADgPwAAAAAAAOk/AAAAAAAA8j8A
AAAAID4PwAAAAAAAABAAAAAAAABABEAAAAAAAAAJQAAAAAAAAQA5AAAAAAAAAEkAAAAAAAACAVQAAA
AAAAgBhAAAAAAAAgHEAAAAAAAAAAgQAAAAAAAECJAAAAAAAABAJEAAAAAAAAJAmQAAAAAAAAAClAAAAA
AACQK0AAAAAAAAEAuQAAAAAAAAiDBAAAAAAAAAAMkAAAAAAAAIgzQAAAAAAAAIDVAAAAAAAADINkAAAAAA
AIA4QAAAAAAAASDpAAAAAAAAAgPEAAAAAAAAAAg+QAAAAAAAAAEBAAAAAAAAAAIPkAAAAAAAACA8QAAAAAAAA

...

mDBAAAAAAABgLkAAAAAAAALArQAAAAAAAAIClAAAAAAAACwJkAAAAAAAAGAkQAAAAAAAAMCJAAAAAAAAAAg
IEAAAAAAAAGAcQAAAAAAAAwBhAAAAAAAABgFUAAAAAAAAEASQAAAAAAAAwA5AAAAAAAACACUAAAAAAAAAMAE
QAAAAAAAgABAAAAAAAACA+T8AAAAAAAADzPwAAAAAAAAOs/AAAAAAAAAA4j8AAAAAAAADWPwAAAAAAAAMg/
AAAAAAAAuD8=
</grid_function>
</fpmd:function3d>
```