

Annotated sample XML schema (file sample.xsd)

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

XML header

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

  <annotation>
    <documentation> $Id: sample.xsd,v 1.12 2008/03/07 20:05:01 fgygi Exp $
      http://www.quantum-simulation.org
      FPMD sample XML Schema specification.
      Copyright (c) 2006-2008 The Regents of the University of California.
    </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 sample Schema specification. In the present example, the version is 1.12.

Include species.xsd

```
<include schemaLocation="species.xsd"/>
```

The included file “species.xsd” contains the XML Schema for species documents, i.e. documents describing atomic species and pseudopotentials. It is included in the sample XML Schema since <species> elements are used in <sample> elements.

<sample> element

```
<element name="sample" type="fpmd:sampleType"/>
<complexType name="sampleType">
  <sequence>
    <element name="description" type="string" minOccurs="0" maxOccurs="1"/>
    <element name="atomset" type="fpmd:atomsetType" minOccurs="0"/>
    <element name="wavefunction" type="fpmd:wavefunctionType" minOccurs="0"/>
    <element name="wavefunction_velocity"
      type="fpmd:wavefunctionType" minOccurs="0"/>
  </sequence>
</complexType>
```

This section defines the <sample> element as a sequence of a <description> element, an <atomset> element, a <wavefunction> element and a <wavefunction_velocity> element. All these sub-elements are optional. The <description> element can contain any information about the sample in the form of a

character string of arbitrary length (it can include newline characters). This is the place to put information about the code that generated the sample, the date of creation, and any code-specific parameters that were used to generate the sample. There is no constraint on the contents of this element (apart from the XML rules regarding character strings). The `<atomset>`, `<wavefunction>` and `<wavefunction_velocity>` elements are declared to be of type `atomsetType` and `wavefunctionType`. These types are described below.

atomsetType definition

```
<complexType name="atomsetType">
  <sequence minOccurs="0">
    <element name="unit_cell" type="fpmd:domainType"
      minOccurs="0"/>
    <element name="species" type="fpmd:speciesType"
      minOccurs="0" maxOccurs="unbounded"/>
    <element name="atom" type="fpmd:atomType"
      minOccurs="0" maxOccurs="unbounded"/>
  </sequence>
  <attribute name="href" type="anyURI" use="optional"/>
</complexType>
```

The `<atomset>` element is of type `atomsetType`. It is used to define the unit cell parameters, the atomic species name, and the atomic positions and velocities. An `<atomset>` is defined as a sequence of a `<unit_cell>` element followed by an arbitrary number of `<species>` elements, and an arbitrary number of `<atom>` elements. An optional attribute can be used to replace the contents of the `<atomset>` with a link to another document. [Note to implementers: The contents of the `<atomset>` elements should be ignored if an `href` attribute is present.] The `speciesType` is defined in the `species.xsd` document which is included in this document using the `<include>` element described above.

atomType definition

```
<
complexType name="atomType">
  <sequence>
    <element name="position" type="fpmd:d3vectorType"/>
    <element name="velocity" minOccurs="0" type="fpmd:d3vectorType"/>
  </sequence>
  <attribute name="name" type="NMTOKEN" use="required"/>
  <attribute name="species" type="NMTOKEN" use="required"/>
</complexType>
```

The `<atom>` element is of type `atomType`. An `<atom>` element must have a `<position>` element and can optionally have a `<velocity>` element. Both `<position>` and `<velocity>` are 3-vectors, defined in the type `d3vectorType` below. The `<atom>` element must have a `name` attribute, and must have a `species` attribute. The atom name and species must be valid html NMTOKENs. This means that they must contain only alphanumeric characters and numbers, and must not start with a number. The most commonly used atom names are made of the element symbol followed by a number (e.g. “Na17”), although any valid NMTOKEN sequence is admissible.

wavefunctionType definition

```
<complexType name="wavefunctionType">
  <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="slater_determinant" type="fpmd:slater_determinantType"
      maxOccurs="unbounded"/>
  </sequence>
  <attribute name="ecut" type="fpmd:nonNegativeDouble" use="optional"/>
  <attribute name="nspin" type="fpmd:nspinType" use="required"/>
  <attribute name="nel" type="nonNegativeInteger" use="required"/>
  <attribute name="nempty" type="nonNegativeInteger" default="0"/>
  <attribute name="href" type="anyURI" use="optional"/>
</complexType>
```

Both the `<wavefunction>` and `<wavefunction_velocity>` elements are of type `wavefunctionType`. A `<wavefunction>` element consists of a `<domain>` element delimiting the region of space on which the wavefunctions are defined. This domain may or may not correspond to the unit cell defined in the `<atomset>` element. The freedom to define the wavefunction domain independently of the atomset unit cell is given to allow for situations in which only a part of the system is described quantum mechanically. The optional `<reference_domain>` element defines a domain that encloses the `<domain>` during variable cell molecular dynamics simulations. The `<grid>` element defines a grid covering the `<domain>`. A `<wavefunction>` element contains at least a `<slater_determinant>` element. Each `<slater_determinant>` defines the one-electron wavefunctions at a given k-point and for a given spin. The optional `<ecut>` element is given as a hint for plane-wave codes to specify the size of a plane-wave basis that accomodates the dimensions of the `<grid>`. The remaining elements specify the total number of spin components of the wavefunction, the total number of electrons and the number of empty states.

domainType

```
<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 `domainType` type consists of three 3-dimensional vectors and is used to define domains in real space.

gridType

```
<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 `gridType` type consists of three integers that define a grid in 3-dimensional space.

slater_determinantType

```
<complexType name="slater_determinantType">
  <sequence minOccurs="0">
    <element name="density_matrix" type="fpmd:density_matrixType"/>
    <element name="grid_function" type="fpmd:grid_functionType"
      maxOccurs="unbounded"/>
  </sequence>
  <attribute name="spin" type="fpmd:spinType" use="optional"/>
  <attribute name="kpoint" type="fpmd:d3vectorType" use="required"/>
  <attribute name="weight" type="double" use="required"/>
  <attribute name="size" type="positiveInteger" use="required"/>
  <attribute name="href" type="anyURI" use="optional"/>
</complexType>
```

A `<slater_determinant>` element is a collection of `<grid_function>` elements, and describes a set of one-particle orbitals. It includes a `<density_matrix>` element that contains occupation numbers. The `spin`, `kpoint`, `weight` and `size` attributes further define the `<slater_determinant>` element.

nspinType

```
<simpleType name="nspinType">
  <restriction base="integer">
    <minInclusive value="1"/>
    <maxInclusive value="2"/>
  </restriction>
</simpleType>
```

spinType

```
<simpleType name="spinType">
  <restriction base="string">
    <enumeration value="up"/>
    <enumeration value="down"/>
  </restriction>
</simpleType>
```

d3vectorType

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

vectorType

```
<complexType name="vectorType">
  <simpleContent>
    <extension base="string">
      <attribute name="type" type="fpmd:numericType" use="required"/>
      <attribute name="size" type="positiveInteger" use="required"/>
      <attribute name="encoding" type="fpmd:encodingType" use="required"/>
    </extension>
  </simpleContent>
</complexType>
```

numericType

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

encodingType

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

grid_functionType

```
<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>
```

A `<grid_function>` element defines a one-electron orbital by giving its value on a subset of the `<grid>` defined in the `<wavefunction>` 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 orbital is defined. 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));
```

doubleListType

```
<simpleType name="doubleListType">
  <list itemType="double"/>
```

```
</simpleType>
```

density_matrixType

```
<complexType name="density_matrixType">
  <simpleContent>
    <extension base="fpmd:doubleListType">
      <attribute name="form" type="fpmd:density_matrix_formType" use="required"/>
      <attribute name="size" type="positiveInteger" use="required"/>
      <attribute name="href" type="anyURI" use="optional"/>
    </extension>
  </simpleContent>
</complexType>
```

The `<density_matrix>` element specifies occupation numbers. It can be given either in full form or in diagonal form. In the diagonal form, only the diagonal elements are given. The body of a `<density_matrix>` element consists of a list of text formatted double precision numbers.

density_matrix_formType

```
<simpleType name="density_matrix_formType">
  <restriction base="string">
    <enumeration value="full"/>
    <enumeration value="diagonal"/>
  </restriction>
</simpleType>
```

This type is used to specify the format of the density matrix (full or diagonal).

```
</schema>
```