Rock.XML v1.0

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XML structure for rock physics models

This document describes the structure of an XML file, referred to as ROCK.XML, which defines a rock; its components, how it is composed and under which reservoir conditions.

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INTRODUCTION

The idea behind the ROCK.XML is to be able to model the density and elastic properties of a fluid-filled rock in a very flexible way, by selecting from and possibly combining many different theories. In order to do this, we need some basic building blocks. The basic building blocks here are fluids, solids, dry rocks (a solid with porosity, but no fluid) and rocks (a combination of solid and fluid).

Each time a building block is defined, it is given a unique identifying name using the `<label>` keyword. This is followed by a keyword specifying which theory we use for building this element, and inside that keyword block, the required parameters for the theory are given. By convention all keywords are written in lowercase only, and with hyphen substituted for space and &, so e.g. Batzle & Wang for calculating brine properties becomes `<batzle-wang-brine>`.

Whenever a solid, fluid or rock is required, we can define it using the `<label>` and theory mechanism. However, if we want to use an element that is already defined, we can use the keyword `<use>` instead of `<label>`, followed by the unique name of the element. Thus, we can easily reuse elements once they are defined. To improve readability, we also include a command for predefining elements.

ROCK.XML is written in the XML language. A two minutes introduction to XML can be seen in this video: http://www.youtube.com/watch?v=QLYf9VgWjmE. This document contains the supported syntax for ROCK.XML.

Note that in XML documents, one can write comments like this <!-- Write your comment here -->. The comments will be ignored by the program reading and processing the XML file.

STRUCTURE

The base structure of ROCK.XML consists of a label, volume, reservoir, evolution, predefinition and rock element, each of which contains sub-elements. This is shown below, without the sub-elements:

```
<label>
<volume>
  ...
</volume>
<trend-cube>
  ...
</trend-cube>
<reservoir>
  ...
</reservoir>
<evolution>
...
</evolution>

<predefinitions>
  ...
</predefinitions>
```

```
<rock>
  ...
</rock>
```

The sub-elements will be basic building blocks (e.g. solid, fluid, dry-rock), properties (e.g. temperature, pore-pressure, density, etc) and theories.

<title>

<label> contains an identifying name for the model.

Below is an example of how <title> can be defined:

```
<title> My model </title>
```

<volume>

<volume> contains properties which are sampled over to calculate multiple realisations of the rock physics model. Each property is defined as an axis of freedom, making up an N-dimensional volume where N is the number of listed properties. Any property defined inside <volume> overrides specifications of an element with identical <label> in the rest of the document.

Inside <volume>, the various properties are listed with the command <axis>.

Below is an example of how <volume> can be defined:

```
<volume>
      <axis>
            <label> CO2 saturation </label>
            <range>
                  <min> 0 </min>
                  <max> 1 </max>
                  <steps> 5 </steps>
            </range>
      </axis>

      <axis>
            <label> total porosity </label>
            <range>
                  <min> 0 </min>
                  <max> 0.4 </max>
                  <steps> 3 </steps>
            </range>
      </axis>
</volume>
```

As shown in the example above, after <axis> follows the commands <label> and <range>.

<range>

The <range> can be defined in two ways. Its entities can either be specified directly or as constant increments.

To specify the entities explicitly, use the <list> keyword with the values given within square brackets.

The constant increment method takes three parameters. The first two are <min> and <max> values, and the third is <steps>, which specifies the number of values the list should have including the minimum and maximum values.

Below is an example demonstrating the range assignments:

```
<range>
  <list> [0 0.1 0.2 0.23 0.27 0.3 0.4] </list>
</range>

<range>
  <min> 0 </min>
  <max> 1 </max>
  <steps> 26 </steps>
</range>
```

<trend-cube>

<trend-cube> contains the trend cubes that can be used for defining a trend on the variables. Each variable defined by a trend may be related to one or two trend cubes. These trend cubes may for example be related to time and depth, and they need to be defined in the entire inversion volume.

<reservoir>

<reservoir> contains reservoir properties, such as pressure, temperature, porosity, fluid saturation, lithology, etc. Reservoir properties given under the keyword <reservoir> are parameters common for all fluids, solids, dry rocks and rocks. For models that depend on these parameters, the values given under reservoir can be used, although they may be overridden locally. The elements <reservoir> are defined by labels to be referred to with the <reservoir-variable> statement. Hence, they must be unique.

After <reservoir>, the command <variable> follows.

Below is an example of how <reservoir> can be defined:

```
<reservoir>
  <variable>
    <label> temperature </label>
    <value> 50 </value>
  </variable>

  <variable>
    <label> total-porosity </label>
    <gaussian>
      <mean> 0.5 </mean>
      <variance> 0.1 </variance>
    </gaussian>
  </variable>

  <variable>
    <label> divided-porosity </label>
    <divide>
```

```
      <divident>
        <reservoir-variable> total-porosity </reservoir-variable>
      </divident>
      <divisor>
        <reservoir-variable> critical-porosity </reservoir-variable>
      </divisor>
    </divide>
  </variable>
</reservoir>
```

<evolution>

The keyword <evolution> groups a set of <evolve> commands. These controls the time development of the reservoir variables. Each variable that evolves in time is controlled by its own <evolve> block. Under the keyword <evolve>, <reservoir-variable>, <one-year-correlation> and <vintage> are given. <reservoir-variable> needs to be the label of one of the variables defined in <reservoir>. <one-year-correlation> defines the correlation between the reservoir variable at two following years. <vintage> is repeated for each vintage of the time development. In <vintage>, <distribution> and <vintage-year> are given. Here, <distribution> is the distribution of the reservoir variable at the given vintage, and it needs to be one of the distributions given under Properties. <vintage-year> is the year of the given vintage of the reservoir variable.

Below is an example with <evolution> for the reservoir variable porosity:

```
<evolution>
  <evolve>
    <reservoir-variable> porosity </reservoir-variable>
    <one-year-correlation> 0.7 </one-year-correlation>
    <vintage>
      <distribution>
        <beta>
          <mean> 0.1 </mean>
          <variance> 0.01 </variance>
        </beta>
      </distribution>
      <vintage-year> 2000 </vintage-year>
    </vintage>

    <vintage>
      <distribution>
        <beta>
          <mean> 0.08 </mean>
          <variance> 0.01 </variance>
        </beta>
      </distribution>
      <vintage-year> 2002 </vintage-year>
    </vintage>
  </evolve>
</evolution>
```

<predefinitions>

<predefinitions> is used for specifying and calculating the elastic properties of basic building blocks, being fluids, solids, dry rocks, or elements and mixtures of these. It will typically use properties specified under <reservoir>. Under the keyword <predefinitions>, fluids, solids and dry rocks are defined for later use, to make the file more readable. After <predefinitions>, one of the commands <fluid>, <solid> or <dry-rock> needs to follow. To be able to use a predefined property other places than where it is defined, the property must be given a unique identification using the <label> statement. It can then be referred to with the <use> statement.

The significant difference between elements in <reservoir> and <predefinitions> is that each element in <reservoir> defines a single property, while it defines an object with several properties in <predefinitions> (e.g. bulk modulus, shear modulus and density). These objects are typically used as inputs to various theories for calculating the effective properties of a mixed material.

<rock>

<rock> contains the final composition of the rock, and will typically use details specified in <reservoir> and <predefinitions>. The <rock> command is followed by either <label> or <use>. If <label> is used, the next keyword is a theory.

Below is an example of a rock composed of a dry rock with fluid introduced using the Gassmann theory (Gassmann 1951):

```
<rock>
  <label> effective rock </label>
  <gassmann>
    <dry-rock>
      <use> quality sand </use>
    </dry-rock>
    <fluid>
      <use> brine </use>
    </fluid>
  </gassmann>
</rock>
```

PROPERTIES

All the properties and function parameters can use previously assigned values in <reservoir>, or be assigned values directly in <predefinitions>. The possible types of value assignments are value, trend, distribution, operator or range.

Value

The simplest form of deterministic value assignment is a single value. For the variables in <reservoir>, the value is given by the command <value>, while it may be given directly for the variable commands of <predefinitions>. Below is an example for each of these cases:

```
<reservoir>
  <variable>
```

```
    <label> temperature </label>
    <value> 40 </value>
  </variable>
</reservoir>

<predefinitions>
  <solid>
    <label> clay </label>
    <tabulated>
      <bulk-modulus> 21 </bulk-modulus>
      <shear-modulus> 7 </shear-modulus>
      <density> 2.6 </density>
    </tabulated>
  </solid>
</predefinitions>
```

Distributions

ROCK.XML supports three distribution functions for assigning probabilistic values to a variable, namely <gaussian>, <beta> and <beta-end-mass>. Whenever several building blocks use the same stochastic variable defined under <reservoir>, the same sample of the variable is used for all the building blocks.

<gaussian>

The Gaussian distribution is defined by the keyword <gaussian>, followed by the distribution parameters <mean> and <variance>.

Below is an example showing the Gaussian distribution function:

```
<reservoir>
  <variable>
    <label> total-porosity </label>
    <gaussian>
      <mean> 0.25 </mean>
      <variance> 0.05 </variance>
    </gaussian>
  </variable>
</reservoir>
```

<beta>

The beta distribution is defined by the keyword <beta>, followed by the distribution parameters <mean>, <variance>, <lower-limit> and <upper-limit>. The beta distribution is defined on the interval [0,1] by default if the upper and lower limits are not given. The mean and variance must be given such that the resulting beta variable is within the given interval.

Below is an example showing the beta distribution function:

```
<reservoir>
  <variable>
    <label> sand lithology </label>
    <beta>
      <mean> 0.2 </mean>
      <variance> 0.1 </variance>
```

```
    </beta>
  </variable>
</reservoir>
```

<beta-end-mass>

The beta distribution with end mass is a Beta distribution combined with a point mass in each end. The variable is in the low end of the distribution with probability <lower-probability> and in the high end with <upper-probability>. The distribution is defined by the keyword <beta-end-mass>, followed by the distribution parameters <mean>, <variance>, <lower-limit>, <upper-limit>, <lower-probability> and <upper-probability>. The beta distribution with end mass is defined on the interval [0,1] by default if the upper and lower limits are not given. The mean and variance must be given such that the resulting beta variable is within the given interval.

Trend

The values of the variables may be given by a trend. The trends are named <trend-1d> or <trend-2d>, with the 1d and 2d endings telling if the property values should be related to one or two trend cubes. These trend cubes may for example be related to time and depth, and they need to be defined in the entire inversion volume. If the trend is to be used, trend cubes must be given on the same level as <reservoir> using the command <trend-cube> following the example below.

```
<reservoir>
  <variable>
    <label> temperature </label>
    <trend-1d>
      <file-name> trend1d.txt </file-name>
      <reference-parameter> time </reference-parameter>
    </trend-1d>
  </variable>

  <variable>
    <label> porosity </label>
    <trend-2d>
      <file-name> trend2d.txt </file-name>
      <reference-parameter-first-axis> time
      </reference-parameter-first-axis>
      <reference-parameter-second-axis> depth
      </reference-parameter-second-axis>
    </trend-2d>
  </variable>
</reservoir>

<trend-cube>
  <parameter-name> time </parameter-name>
  <file-name> trend_cube_time.txt </file-name>
</trend-cube>

<trend-cube>
  <parameter-name> depth </parameter-name>
```

```
  <file-name> trend_cube_depth.txt </file-name>
</trend-cube>
```

Operator

The operators are listed below.

<divide>

This is a mathematical division of two numbers (dividend/divisor). The operator takes two parameters; <dividend> and <divisor>.

Below is an example of calculating the volume fraction of the mineral constituent from the total and critical porosity:

```
<reservoir>
  <variable>
    <label> mineral constituent volume fraction </label>
    <divide>
      <dividend>
        <reservoir-variable> total-porosity </reservoir-variable>
      </dividend>
      <divisor>
        <reservoir-variable> critical-porosity </reservoir-variable>
      </divisor>
    </divide>
  </variable>
</reservoir>
```

<multiply>

This is a multiplication of several factors (<factor>*<factor>…*<factor>). The operator takes two or more <factor> parameters.

Below is an example using <multiply> to convert pressure from GPa to MPa:

```
<reservoir>
  <variable>
    <label> MPa pressure </label>
    <multiply>
      <factor>
        <reservoir-variable> GPa pressure </reservoir-variable>
      </factor>
      <factor> 1000 </factor>
    </multiply>
  </variable>
</reservoir>
```

CONSTITUENTS

The constituents are the basic building blocks used to compose a rock. These basic building blocks are fluids, solids and dry rocks, being a solid with porosity but no fluid. Whenever a constituent is required in a theory, we can define it using a <label> followed by a theory. However, if we want to use a constituent that is already defined, we use the keyword <use> instead of <label>, followed

by the unique name of the element. Thus, constituents can easily be used over and over once they are defined.

Basic building blocks

Each time a building block is defined, it is given a unique identifying name using the <label> keyword. This is followed by a keyword specifying which theory we use for building this constituent. The basic building blocks are <fluid>, <solid> and <dry-rock>.

<fluid>

Fluids are generally defined by the command <fluid>. The fluid command is followed either by the command <label> to specify a new fluid, or <use> to use a predefined fluid. In the latter case, the fluid is now done; in the former case, the next keyword is the theory used to model the fluid.

Below is an example of brine defined using Batzle and Wang's theory (1992):

```
<predefinitions>
  <fluid>
    <label> brine </label>
    <batzle-wang-brine>
      <pore-pressure> 20 </pore-pressure>
      <temperature> 60 </temperature>
      <salinity> 0.05 </salinity>
    </batzle-wang-brine>
  </fluid>
</predefinitions>
```

<solid>

Solids follow the same pattern as fluids, with <solid> as the defining keyword, followed by <label>, and the following keyword defining the theory used. As with fluids, <use> can be used instead of <label>, to use a previously specified solid.

Below is an example of quartz defined using tabulated values. (See more about tabulated values under Theories):

```
<predefinitions>
  <solid>
    <label> quartz </label>
    <tabulated>
      <bulk-modulus> 37 </bulk-modulus>
      <shear-modulus> 44 </shear-modulus>
      <density> 2.65 </density>
    </tabulated>
  </solid>
</predefinitions>
```

<dry-rock>

Dry rocks are a particular type of solid, as they have a defined porosity, yet no fluids added, so they are not rocks according to the rock-definition in ROCK.XML. In addition to the density and effective elastic moduli for the specified porosity, they also contain information about the effective mineral properties.

Dry rocks are specified with <dry-rock>, followed by <label> or <use>. If <label> is given, it is followed by a theory for calculating the effective elastic moduli. An implicit part of the theories is that the density is calculated using the arithmetic average of the constituents.

Below is an example of a sandstone dry rock:

```
<predefinitions>
  <dry-rock>
    <label> porous sandstone </label>
    <hill>
      <constituent>
        <solid>
          <use> quartz </use>
        </solid>
        <volume-fraction> 0.3 </volume-fraction>
      </constituent>
      <constituent>
        <dry-rock>
          <use> Walton high porous sandstone </use>
        </dry-rock>
      </constituent>
    </hill>

  </dry-rock>
</predefinitions>
```

Theories

Each time a basic building block constituent is defined, it is given a unique name followed by a keyword specifying which theory we use for building this element. Inside the theory block, the required parameters for the theory are given.

The theories are used for calculating the bulk and shear moduli. In addition, they are implicitly used for calculating the density using the arithmetic average of the constituent densities.

The following is a list of theories which can be used in ROCK.XML.

<batzle-wang-brine>

The theory of Batzle and Wang (1992) can be used for calculating the brine properties.

List of parameters.

Parameter	Type/Unit	Details
<pore-pressure>	MPa	
<temperature>	℃	
<salinity>	Fraction of 1	Salinity of 5%: <salinity>0.05</salinity>

Below is an example where two types of brines are defined:

```
<predefinitions>
  <fluid>
    <label> brine 1 </label>
    <batzle-wang-brine>
      <pore-pressure>
        <reservoir-variable> pore-pressure </reservoir-variable>
      </pore-pressure>
      <temperature>
        <reservoir-variable> temperature </reservoir-variable>
      </temperature>
      <salinity> 0.05 </salinity>
    </batzle-wang-brine>
  </fluid>

  <fluid>
    <label> brine 2 </label>
    <batzle-wang-brine>
      <pore-pressure> 20 </pore-pressure>
      <temperature> 60 </temperature>
      <salinity> 0.05 </salinity>
    </batzle-wang-brine>
  </fluid>
</predefinitions>
```

<span-wagner-co2>

The theory of Span and Wagner (1996) can be used for calculating the CO2 properties.

List of parameters.		
Parameter	**Type/Unit**	**Details**
<pressure>	MPa	
<temperature>	°C	

Below is an example where two types of brines are defined:

```
<predefinitions>
  <fluid>
    <label> co2 1 </label>
    <span-wagner-co2>
      <pore-pressure> 10 </pore-pressure>
      <temperature> 36 </temperature>
    </span-wagner-co2>
  </fluid>
</predefinitions>
```

<bounding>

The bounding model is a mixing model between a stiff and soft end-member of the rock. The stiff end-member is calculated mixing the stiffer constituents using the Voigt model (Voigt 1928). The soft end-member is calculated mixing the softer constituents using the Reuss model (Reuss 1929).

The bounding model can only be used to make a rock, i.e. inside the <rock> element.

List of parameters. (Optional parameters are prefixed with *).		
Parameter	**Type/Unit**	**Details**
<upper-bound>		Given by <rock>. The rock should follow a Voigt model mixing a fluid and a solid.
<lower-bound>		Given by <rock>. The rock should follow a Reuss model mixing a fluid and a solid.
<porosity>		Porosity of the bounding rock. The porosity of the Bounding model should be the same variable as <volume-fraction> of the fluid in the Reuss and Voigt models where a solid and fluid are mixed, and it should be declared in <reservoir>. If the porosity is not the same variable as the volume fractions, <porosity> overrides the volume fractions. The porosity is uncorrelated with the weights.
<bulk-modulus-weight>		The bulk modulus is calculated using the weights and upper/lower bounds from the relation $K = W_k$ x *upper-bound* + (1- W_k) x *lower-bound*. Higher weights therefore indicate stiffer rock, while lower weights indicate softer rock.
<p-wave-modulus-weight>		The p-wave modulus is often termed M, and calculated from the relation M = density x Vp^2. The p-wave modulus is calculated using the weights and upper/lower bounds from the relation $M = W_m$ x *upper-bound* + (1 - W_m) x *lower-bound*. Higher weights therefore indicate stiffer rock, while lower weights indicate softer rock.
<correlation-weights>		The correlation between the bulk-modulus weight and p-wave-modulus-weight. Default 0.

Below is an example where the bounding model is defined:

```
<rock>
  <label> bounding-rock </label>
  <bounding>
    <upper-bound>
      <rock>
        <label> upper-rock </label>
        <voigt>
          <label> voigt </label>
          <constituent>
            <fluid>
              <use> brine </use>
            </fluid>
            <volume-fraction>
              <reservoir-variable> porosity </reservoir-variable>
            </volume-fraction>
          </constituent>
          <constituent>
            <solid>
              <use> quartz </use>
            </solid>
          </constituent>
        </voigt>
      </rock>
    </upper-bound>
    <lower-bound>
      <rock>
        <label> lower-rock </label>
        <reuss>
          <label> reuss </label>
          <constituent>
            <fluid>
              <use> oil </use>
            </fluid>
            <volume-fraction>
              <reservoir-variable> porosity </reservoir-variable>
            </volume-fraction>
          </constituent>
          <constituent>
            <solid>
              <use> clay </use>
            </solid>
          </constituent>
        </reuss>
      </rock>
    </lower-bound>
    <porosity>
      <reservoir-variable> porosity </reservoir-variable>
    </porosity>
    <bulk-modulus-weight>
      <gaussian>
        <mean> 0.5 </mean>
        <variance> 0.01 </variance>
```

```
      </gaussian>
    </bulk-modulus-weight>
    <p-wave-modulus-weight>
      <gaussian>
        <mean> 0.4 </mean>
        <variance> 0.01 </variance>
      </gaussian>
    </p-wave-modulus-weight>
    <correlation-weights> 0.8 </correlation-weights>
  </bounding>
</rock>
```

<dem>

Differential effective medium (DEM) theory (Bruggeman 1935; Berryman 1992; Berryman 1995) is an inclusion based model. One of the constituents acts as the host material while the other constituents are treated as inclusions. In addition to volume fractions of the inclusions, their pore geometry must be specified. Typical use of DEM is mixing two solids, adding empty pores to a solid ("later" saturated using Gassmann theory) or adding fluid filled pores in a solid directly. Note that this is an asymmetric model, where interchanging host and constituent typically leads to different solutions.

List of parameters. (Optional parameters are prefixed with *).		
Parameter	**Type/Unit**	**Details**
<host>		Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>
<inclusion>		Given by <fluid>, <solid> or <dry-rock> followed by <aspect-ratio> and <volume-fraction>
*...		
*<inclusion>		Given by <fluid>, <solid> or <dry-rock> followed by <aspect-ratio>.

Note that inclusions beyond the first one are optional. Like in the example below, the same material can be used in all inclusions, just that they have different geometries. But it is also possible to use different materials for the various inclusions. One of the <volume-fraction> keywords should be left out, as this is calculated according to 1 – {volume-fraction of the other hosts and inclusions}. Whenever more than one inclusion is given, the volume fractions cannot be trends or distributions.

Below is an example where DEM is first used to mix two solids and then to include vacuum pores (20% porosity):

```
<predefinitions>
  <solid>
    <label> effective mineral </label>
```

```
    <dem>
      <host>
        <solid>
          <use> quartz </use>
        </solid>
        <volume-fraction>
          <reservoir-variable> Q vol fract </reservoir-variable>
        </volume-fraction>
      </host>
      <inclusion>
        <solid>
          <use> clay </use>
        </solid>
        <aspect-ratio> 0.01 </aspect-ratio>
      </inclusion>
    </dem>
  </solid>

  <dry-rock>
    <label> example using DEM porous shaley sand </label>
    <dem>
      <host>
        <solid>
          <use> sandstone effective mineral </use>
        </solid>
        <volume-fraction>
          <reservoir-variable> mineral constituent volume fraction
          </reservoir-variable>
        </volume-fraction>
      </host>
      <inclusion>
        <fluid>
          <use> empty </use>
        </fluid>
        <aspect-ratio> 0.2 </aspect-ratio>
        <volume-fraction> 0.15 </volume-fraction>
      </inclusion>
      <inclusion>
        <fluid>
          <use> empty </use>
        </fluid>
        <aspect-ratio> 0.1 </aspect-ratio>
        <volume-fraction> 0.05 </volume-fraction>
      </inclusion>
    </dem>
      </dry-rock>
</predefinitions>
```

<gassmann>

The theory of Gassmann (1951) can be used for calculating the effective elastic properties of rock when substituting one fluid with another. Here, it is restricted to the case of replacing empty pores with some type of fluid (liquid or gas).

List of parameters.		
Parameter	**Type/Unit**	**Details**
<dry-rock>	Dry-rock	Given by <use> or <label> and theory construction
<fluid>	Fluid	Given by <use> or <label> and theory construction

Note that the software will extract details about the effective mineral properties and porosity which are required in addition to the explicitly provided information, to calculate the effective elastic properties of the fluid saturated rock. These are taken from the dry rock component.

Below is an example of a fluid introduced in a dry rock using the Gassmann theory:

```
<rock>
  <label> effective rock </label>
  <gassmann>
    <dry-rock>
      <use> dry rock </use>
    </dry-rock>
    <fluid>
      <use> effective fluid </use>
    </fluid>
  </gassmann>
</rock>
```

<hashin-shtrikman-walpole-low> or <hsw-low>

Used for calculating the Hashin-Shtrikman-Walpole lower bound (Walpole 1966a,b; Hashin & Shtrikman 1963); the theoretical lower limit of effective moduli for an isotropic mixture. It can for example be used to model a mixture of a soft and stiff mineral where the soft mineral acts as a surrounding shell around the stiffer mineral. Walpole extended the theory of Hashin-Shtrikman by not constraining the bulk and shear moduli of the stiffer material to both be larger than that of the soft material.

List of parameters.		
Parameter	**Type/Unit**	**Description**
<constituent>	Solid, fluid or dry-rock	Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*
<constituent>	Solid, fluid or dry-rock	Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*

*One of the <volume-fraction> keywords should be left out, as this is calculated according to 1 – {volume-fraction of the other hosts and inclusions}. Whenever more than one inclusion is given, the volume fractions cannot be trends or distributions.

The parameter order of stiff and soft constituents is arbitrary.

Example of <hsw-low> used on two solids:

```
<predefinitions>
  <solid>
    <label> clay coating quartz </label>
    <hsw-low>
      <constituent>
        <solid>
          <use> quartz </use>
        </solid>
        <volume-fraction> 0.8 </volume-fraction>
      </constituent>
      <constituent>
        <solid>
          <use> clay </use>
        </solid>
      </constituent>
    </hsw-low>
  </solid>
</predefinitions>
```

<hashin-shtrikman-walpole-up> or <hsw-up>

Used for calculating the Hashin-Shtrikman-Walpole upper bound (Walpole 1966a,b; Hashin & Shtrikman 1963); the theoretical upper limit of effective moduli for an isotropic mixture. It can for example be used to model a mixture of a soft and stiff mineral where the stiff mineral acts as a surrounding shell around the softer mineral. Walpole extended the theory of Hashin-Shtrikman by not constraining the bulk and shear moduli of the stiffer material to both be larger than that of the soft material.

List of parameters.

Parameter	Type/Unit	Description
<constituent>	Solid, fluid or dry-rock	Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*
<constituent>	Solid, fluid or dry-rock	Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*

*One of the <volume-fraction> keywords should be left out, as this is calculated according to 1 – {volume-fraction of the other hosts and inclusions}. Whenever more than one inclusion is given, the volume fractions cannot be trends or distributions.

The parameter order of stiff and soft constituents is arbitrary.

Example of <hsw-up> used on two solids:

```
<predefinitions>
  <solid>
    <label> quarts coating clay </label>
    <hsw-up>
      <constituent>
        <solid>
          <use> quartz </use>
        </solid>
        <volume-fraction> 0.8 </volume-fraction>
      </constituent>
      <constituent>
        <solid>
          <use> clay </use>
        </solid>
      </constituent>
    </hsw-up >
  </solid>
</predefinitions>
```

<hill>

Used for calculating the average of <reuss> and <voigt> of various constituents (Hill 1963). Note that <hill> can be used to calculate the effective bulk modulus of a patchy fluid.

List of parameters.		
Parameter	**Type/Unit**	**Description**
<constituent>	Solid, fluid or dry-rock	Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*
…		
<constituent>	Solid, fluid or dry-rock	Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*

*One of the <volume-fraction> keywords should be left out, as this is calculated according to 1 – {volume-fraction of the other hosts and inclusions}. Whenever more than one inclusion is given, the volume fractions cannot be trends or distributions.

Below is an example of <hill> used on two solids:

```
<predefinitions>
  <solid>
    <label> shaley sand </label>
    <hill>
      <constituent>
        <solid>
          <use> quartz </use>
        </solid>
        <volume-fraction> 0.2 </volume-fraction>
```

```
      </constituent>
      <constituent>
        <solid>
          <use> clay </use>
        </solid>
      </constituent>
    </hill>
  </solid>
</predefinitions>
```

<reuss>

Used for calculating the harmonic average of various constituents (Reuss 1929). This is typically used when calculating effective bulk moduli of fluids, then referred to as Wood's theory (Wood 1955). However, for simplicity, ROCK.XML uses <reuss> both for fluid and solids.

List of parameters.		
Parameter	**Type/Unit**	**Description**
<constituent>		Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction> *
…		
<constituent>		Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*

*One of the <volume-fraction> keywords should be left out, as this is calculated according to 1 – {volume-fraction of the other hosts and inclusions}. Whenever more than one inclusion is given, the volume fractions cannot be trends or distributions.

Below is an example of <reuss> used on two fluids:

```
<predefinitions>
  <fluid>
    <label> fizz </label>
    <reuss>
      <constituent>
        <fluid>
          <label> brine </label>
          <batzle-wang-brine>
            <pore-pressure> 20 </pore-pressure>
            <temperature> 60 </temperature>
            <salinity> 0.05 </salinity>
          </batzle-wang-brine>
        </fluid>
        <volume-fraction> 0.95 </volume-fraction>
      </constituent>
      <constituent>
        <fluid>
          <use> gas </use>
```

```
        </fluid>
        </constituent>
    </reuss>
  </fluid>
</predefinitions>
```

<tabulated>

<tabulated> allows specifying properties explicitly. The properties can either be specified by the set <density>, <bulk-modulus> and <shear-modulus>, or by the set <density>, <vp> and <vs>. In case of fluids, <shear-modulus> (or <vs>) is omitted, and is by default 0. The correlation between the variables may also be added. If the correlations are not used, the variables are assumed to have zero correlation.

Only for dry rocks:

Then the <total-porosity> and <mineral-bulk-modulus> (i.e. bulk and shear moduli of the effective mineral) are defined.

List of properties.

Properties	**Type/Unit**	**Description**
<density>	g/cm^3	
<bulk-modulus>	GPa	
<shear-modulus>	GPa	Omitted for fluids (defaults to 0 GPa).
<correlation-bulk-shear>		Optional, default zero
<correlation-bulk-density>		Optional, default zero
<correlation-shear-density>		Optional, default zero
<vp>	km/s	
<vs>	km/s	Can be omitted for fluids (defaults to 0 km/s).
<correlation-vp-vs>		Optional, default zero
<correlation-vp-density>		Optional, default zero
<correlation-vs-density>		Optional, default zero
<total-porosity>		Only for dry rocks

<mineral-bulk-modulus>	GPa	Only for dry rocks

Below is an example for specifying the properties of fluids and solids:

```
<predefinitions>
  <fluid>
    <label> brine </label>
    <tabulated>
      <bulk-modulus> 2.62 </bulk-modulus>
      <density> 1.017 </density>
    </tabulated>
  </fluid>

  <fluid>
    <label> gas</label>
    <tabulated>
      <vp> 0.534 </vp>
      <density> 0.146 </density>
      <correlation-vp-density> 0.4 </correlation-vp-density>
    </tabulated>
  </fluid>

  <solid>
    <label> quartz </label>
    <tabulated>
      <bulk-modulus> 37 </bulk-modulus>
      <shear-modulus> 44 </shear-modulus>
      <density> 2.65 </density>
    </tabulated>
  </solid>

  <solid>
    <label> clay </label>
    <tabulated>
      <vp> 3.81 </vp>
      <vs > 1.88 </vs >
      <density> 2.6 </density>
      <correlation-vp-vs> 0.7 </correlation-vp-vs>
      <correlation-vp-density> 0.4 </correlation-vp-density>
      <correlation-vs-density> 0.3 </correlation-vs-density>
    </tabulated>
  </solid>
</predefinitions>
```

<voigt>

Used for calculating the arithmetic average of various constituents (Voigt 1928).

List of parameters.		
Parameter	**Type/Unit**	**Description**

<constituent>		Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*
…		
<constituent>		Given by <fluid>, <solid> or <dry-rock> followed by <volume-fraction>*

*One of the <volume-fraction> keywords should be left out, as this is calculated according to 1 – {volume-fraction of the other hosts and inclusions}. Whenever more than one inclusion is given, the volume fractions cannot be trends or distributions.

Below is an example of <voigt> used on two solids:

```
<predefinitions>
  <solid>
    <label> shaley sand </label>
    <voigt>
      <constituent>
        <solid>
          <label> quartz </label>
          <tabulated-solid>
            <bulk-modulus> 37 </bulk-modulus>
            <shear-modulus> 44 </shear-modulus>
            <density> 2.65 </density>
          </tabulated-solid>
        </solid>
        <volume-fraction> 0.2 </volume-fraction>
      </constituent>
      <constituent>
        <solid>
          <use> clay </use>
        </solid>
      </constituent>
    </voigt>
  </solid>
</predefinitions>
```

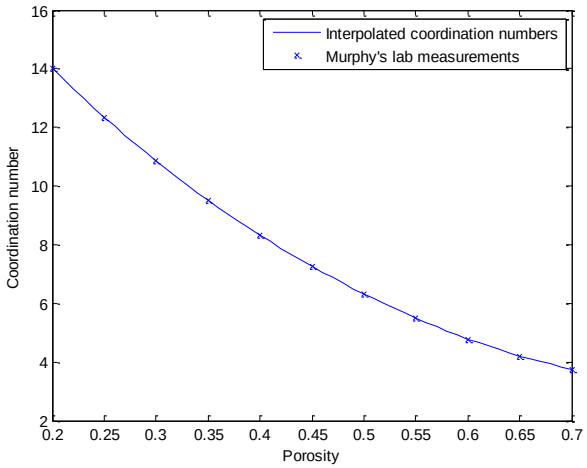
<walton>

The Walton (1987) model is a contact model for spherical grain packing. It assumes the normal and shear deformation of a two-grain-combination occur simultaneously. The effective elastic moduli can be modelled assuming no or a very large friction coefficient. The friction factor can be used to model friction coefficients between these two extremes. In the Walton model the friction only affects the shear modulus.

List of parameters. (Optional parameters are prefixed with *).		
Parameter	**Type/Unit**	**Details**
<solid>	Solid	

<friction>	0.0..1.0	0: no friction, 1: high friction and any value between is an arithmetic average between the two extremes
<pressure>	MPa	Hydrostatic confining pressure (often substituted with effective pressure)
<porosity>	0.0..1.0	
*<coord-nr>		Average contact points per grain. Optional; defaults to interpolated value from porosity and coordination measurements by Murphy (1982)

Note that the dataset by Murphy is between 0.2 and 0.7 porosity and 14.007 and 4.783 in coordination number. Estimated values outside that range are extrapolations.



Example of <walton> used on two solids:

```
<predefinitions>
  <dry-rock>
    <label> unconsolidated granular media </label>
    <walton>
      <solid>
        <use> quartz </use>
      </solid>
      <no-slip> 0.6 </no-slip>
      <pressure> 20 </pressure>
      <porosity>
        <reservoir-variable> critical porosity </reservoir-variable>
      </porosity>
      <coord-nr>
        <reservoir-variable> coord-nr </reservoir-variable>
      </coord-nr>
    </walton>
      </dry-rock>
</predefinitions>
```

EXAMPLES

Below are some examples of rocks defined using ROCK.XML.

"Simple" ROCK.XML based on the Hill model

The solid constituents are quartz and clay, and brine and gas for fluids. The solids are mixed using Hill (1963) and fluids using Reuss (1929). The Hill model is also used for calculating the effective dry rock properties in the porosity range between the mineral point and the high porosity end-member which have been given some tabulated values. The fluid phase is introduced using Gassmann theory (Gassmann 1951).

```
<reservoir>
  <variable>
    <label> total porosity </label>
    <value> 0.3 </value>
  </variable>

  <variable>
    <label> critical porosity </label>
    <value> 0.4 </value>
  </variable>

  <variable>
    <label> gas saturation </label>
    <value> 0.8 </value>
  </variable>

  <variable>
    <label> sand lithology </label>
    <value> 0.6 </value>
  </variable>

  <variable>
    <label> temperature </label>
    <value> 50 </value>
  </variable>

  <variable>
    <label> pore pressure </label>
    <value> 20 </value>
  </variable>

  <variable>
    <label> mineral constituent volume fraction </label>
    <divide>
      <dividend>
        <reservoir-variable> total porosity </reservoir-variable>
      </dividend>
      <divisor>
        <reservoir-variable> critical porosity </reservoir-variable>
      </divisor>
    </divide>
  </variable>
</reservoir>
```

```
<predefinitions>
  <fluid>
    <label> gas </label>
    <tabulated>
      <bulk-modulus> 0.042 </bulk-modulus>
      <density> 0.15 </density>
    </tabulated>
  </fluid>

  <fluid>
    <label> brine </label>
    <batzle-wang-brine>
      <pore-pressure>
        <reservoir-variable> pore pressure </reservoir-variable>
      </pore-pressure>
      <temperature>
        <reservoir-variable> temperature </reservoir-variable>
      </temperature>
      <salinity> 0.05 </salinity>
    </batzle-wang-brine>
  </fluid>

  <fluid>
    <label> effective fluid </label>
    <reuss>
      <constituent>
        <fluid>
          <use> gas </use>
        </fluid>
        <volume-fraction>
          <reservoir-variable> gas saturation </reservoir-variable>
        </volume-fraction>
      </constituent>
      <constituent>
        <fluid>
          <use> brine </use>
        </fluid>
      </constituent>
    </reuss>
  </fluid>

  <solid>
    <label> quartz </label>
    <tabulated>
      <bulk-modulus> 37 </bulk-modulus>
      <shear-modulus> 44 </shear-modulus>
      <density> 2.65 </density>
    </tabulated>
  </solid>

  <solid>
    <label> clay </label>
    <tabulated>
      <bulk-modulus> 21 </bulk-modulus>
```

```
    <shear-modulus> 7 </shear-modulus>
    <density> 2.6 </density>
  </tabulated>
</solid>

<solid>
  <label> effective mineral </label>
  <hill>
    <constituent>
      <solid>
        <use> quartz </use>
      </solid>
      <volume-fraction>
        <reservoir-variable> sand lithology </reservoir-variable>
      </volume-fraction>
    </constituent>
    <constituent>
      <solid>
        <use> clay </use>
      </solid>
    </constituent>
  </hill>
</solid>

<dry-rock>
  <label> high porosity end-member </label>
  <tabulated>
    <density> 2.5 </density>
    <bulk-modulus> 7 </bulk-modulus>
    <shear-modulus> 5.5 </shear-modulus>
     <total-porosity>
       <reservoir-variable> critical porosity </reservoir-variable>
    </total-porosity>
    <mineral-bulk-modulus>
      <use> effective mineral </use>
    </mineral-bulk-modulus>
  </tabulated>

</dry-rock>

<dry-rock>
  <label> dry rock </label>
  <hill>
    <constituent>
      <solid>
        <use> effective mineral </use>
      </solid>
      <volume-fraction>
        <reservoir-variable> mineral constituent volume fraction
        </reservoir-variable>
      </volume-fraction>
    </constituent>
    <constituent>
```

```
        <solid>
          <use> high porosity end-member </use>
        </solid>
      </constituent>
    </hill>
      </dry-rock>
</predefinitions>

<rock>
  <label> effective rock </label>
  <gassmann>
    <dry-rock>
      <use> dry rock </use>
    </dry-rock>
    <fluid>
      <use> effective fluid </use>
    </fluid>
  </gassmann>
</rock>
```

"Complex" ROCK.XML based on the Walton model

The solid constituents are quartz and clay, and brine and gas for fluids. The solids are mixed using Hill (1963) and fluids using Reuss (1929). The differential effective medium model (Bruggemann 1935; Berryman 1992; Berryman 1995) is used for calculating effective dry rock properties in the porosity range between the mineral point and the high porosity end-member which is calculated using Walton's model (Walton 1987). The fluid phase is introduced using Gassmann theory (Gassmann 1951). Here a Gaussian distribution function is applied to the total porosity and a range of values (or alternatively, a uniform distribution) is applied to the gas saturation.

```
<reservoir>
  <variable>
    <label> total porosity </label>
    <gaussian>
      <mean> 0.2 </mean>
      <variance> 0.05 </variance>
    </gaussian>
  </variable>

  <variable>
    <label> pore geometry 1 </label>
    <value> 0.2 </value>
  </variable>

  <variable>
    <label> pore geometry 2 </label>
    <value> 0.05 </value>
  </variable>

  <variable>
    <label> vol fract pore 1 </label>
    <multiply>
      <factor> 0.8 </factor>
```

```
      <factor>
        <reservoir-variable> total porosity </reservoir-variable>
      </factor>
    </multiply>
  </variable>

  <variable>
    <label> vol fract pore 2 </label>
    <multiply>
      <factor> 0.2 </factor>
      <factor>
        <reservoir-variable> total porosity </reservoir-variable>
      </factor>
    </multiply>
  </variable>

  <variable>
    <label> gas saturation </label>
    <uniform>
      <a> 0 </a>
      <b> 1 </b>
    </uniform>
  </variable>

  <variable>
    <label> sand lithology </label>
    <value> 0.6 </value>
  </variable>

  <variable>
    <label> pore pressure </label>
    <value> 20 </value>
  </variable>

  <variable>
    <label> eff. pressure </label>
    <value> 20 </value>
  </variable>


  <variable>
    <label> temperature </label>
    <value> 50 </value>
  </variable>

  <variable>
    <label> critical porosity </label>
    <value> 0.4 </value>
  </variable>

  <variable>
    <label> coord-nr </label>
    <value> 8.3 </value>
  </variable>
```

```
  <variable>
    <label> high friction </label>
    <value> 1 </value>
  </variable>

  <variable>
    <label> mineral constituent volume fraction </label>
    <divide>
      <dividend>
        <reservoir-variable> total porosity </reservoir-variable>
      </dividend>
      <divisor>
        <reservoir-variable> critical porosity
        </reservoir-variable>
      </divisor>
    </divide>
  </variable>
</reservoir>

<predefinitions>
  <fluid>
    <label> gas </label>
    <tabulated>
      <bulk-modulus> 0.042 </bulk-modulus>
      <density> 0.15 </density>
    </tabulated>
  </fluid>

  <fluid>
    <label> brine </label>
    <batzle-wang-brine>
      <pore-pressure>
        <reservoir-variable> pore pressure </reservoir-variable>
      </pore-pressure>
      <temperature>
        <reservoir-variable> temperature </reservoir-variable>
      </temperature>
      <salinity> 0.05 </salinity>
    </batzle-wang-brine>
  </fluid>

  <fluid>
    <label> effective fluid </label>
    <reuss>
      <constituent>
        <fluid>
          <use> gas </use>
        </fluid>
        <volume-fraction>
          <reservoir-variable> gas-saturation </reservoir-variable>
        </volume-fraction>
      </constituent>
      <constituent>
```

```
      <fluid>
        <use> brine </use>
      </fluid>
    </constituent>
  </reuss>
</fluid>

<solid>
  <label> quartz </label>
  <tabulated>
    <bulk-modulus> 37 </bulk-modulus>
    <shear-modulus> 44 </shear-modulus>
    <density> 2.65 </density>
  </tabulated>
</solid>

<solid>
  <label> clay </label>
  <tabulated>
    <bulk-modulus> 21 </bulk-modulus>
    <shear-modulus> 7 </shear-modulus>
    <density> 2.6 </density>
  </tabulated>
</solid>

<solid>
  <label> effective mineral </label>
  <hill>
    <constituent>
      <solid>
        <use> quartz </use>
      </solid>
      <volume-fraction>
        <reservoir-variable> sand lithology </reservoir-variable>
      </volume-fraction>
    </constituent>
    <constituent>
      <solid>
        <use> clay </use>
      </solid>
    </constituent>
  </hill>
</solid>

<dry-rock>
  <label> high porosity end-member </label>
  <walton>
    <solid>
      <use> effective mineral </use>
    </solid>
    <no-slip>
      <reservoir-variable> high friction </reservoir-variable>
    </no-slip>
```

```
      <pressure>
        <reservoir-variable> eff. pressure </reservoir-variable>
      </pressure>
      <porosity>
        <reservoir-variable> critical porosity </reservoir-variable>
      </porosity>
      <coord-nr>
        <reservoir-variable> coord-nr </reservoir-variable>
      </coord-nr>
    </walton>
      </dry-rock>

  <dry-rock>
    <label> dry rock </label>
    <dem>
      <host>
        <solid>
          <use> effective mineral </use>
        </solid>
        <volume-fraction>
          <reservoir-variable> mineral constituent volume fraction
          </reservoir-variable>
        </volume-fraction>
      </host>
      <inclusion>
        <fluid>
          <use> vacuum </use>
        </fluid>
        <aspect-ratio>
          <reservoir-variable> pore geometry </reservoir-variable>
        </aspect-ratio>
        <volume-fraction>
          <reservoir-variable> vol frac pore 1 </reservoir-variable>
        </volume-fraction>
      </inclusion>
      <inclusion>
        <fluid>
          <use> vacuum </use>
        </fluid>
        <aspect-ratio>
          <reservoir-variable> pore geometry 2 </reservoir-variable>
        </aspect-ratio>
      </inclusion>
    </dem>

  </dry-rock>
</predefinitions>

<rock>
  <label> effective rock </label>
  <gassmann>
    <dry-rock>
      <use> dry rock </use>
    </dry-rock>
```

```
    <fluid>
      <use> effective fluid </use>
    </fluid>
  </gassmann>
</rock>
```