User's Manual Version 3.0

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Contents

[1] This feature may not work properly on all systems, although it will always work on Windows systems.

Chapter 1

Introduction

1.1 Overview of FEBio

FEBio is a nonlinear finite element solver that is specifically designed for biomechanical applications. It offers modeling scenarios, constitutive models and boundary conditions that are relevant to many research areas in biomechanics, thus offering a powerful tool for solving 3D problems in computational biomechanics. The software is open-source and the source code, as well as pre-compiled executables for Windows, OS-X and Linux platforms are available for download at http://febio.org. This chapter presents a brief overview of the available features of FEBio.

FEBio can solve different kinds of physics. It can solve problems in structural mechanics, biphasic and multiphasic physics, fluid mechanics, and fluid-solid interaction (FSI). Both (quasi-) static (or steady-state) and dynamic (or transient) analyses can be performed in each of the different physics modules. For instance, in the structural mechanics module, the (quasi-) static response of the system is sought in a quasi-static analysis and the effects of inertia are ignored. In a dynamic analysis, the inertial effects are included in the governing equations to calculate the time dependent response of the system. In the biphasic module, a coupled solid-fluid problem is solved. In a transient biphasic analysis the time dependent response of both the solid and the fluid phase is determined. For the steady-state analysis the final relaxed state is recovered. Similarly, for multiphasic problems, both the time dependent transient response as well as the steady-state response can be determined. For fluid analyses, dynamic and steady-state responses may be specified.

Many nonlinear constitutive models are available, allowing the user to model the often complicated biological tissue behavior. Several isotropic constitutive models are supported such as Neo-Hookean, Mooney-Rivlin, Ogden, Arruda-Boyce and Veronda-Westmann. All these models have a nonlinear stress-strain response and are objective for large deformations. In addition to the isotropic models there are several transversely isotropic and orthotropic constitutive models available. These models exhibit anisotropic behavior in a single or multiple preferred directions and are useful for representing biological tissues such as tendons, muscles, cartilage and other tissues that contain fibers. FEBio also contains a *rigid body* constitutive model. This model can be used to represent materials or structures whose deformation is negligible compared to that of other materials in the overall model. Several constitutive models are available for representing the solid phase of biphasic and multiphasic materials, which are materials that contain both a solid phase and a fluid phase. For incompressible materials FEBio employs special algorithms for enforcing the incompressibility constraint. A three-field formulation is used for tri-linear hexahedral and wedge elements. This algorithm allows the user to capture the accurate response of highly

incompressible materials.

FEBio can now also solve first-order computational homogenization problems. In such problems, the response of the macro-model is determined by the averaged local response of a representative volume element (RVE). The deformation of the macro-model, and more specifically the local deformation gradient, is applied to a RVE model which in turns determines the stress (and tangent) of the macro-model.

FEBio supports a wide range of boundary conditions and loads to model interactions between materials that are relevant to problems in biomechanics. Deformable models can be connected to rigid bodies. With this feature, the user can model prescribed rotations and torques for rigid segments, thereby allowing the coupling of rigid body mechanics with deformable continuum mechanics. FEBio provides the ability to represent frictionless and frictional contact between rigid and/or deformable materials using sliding interfaces. A sliding surface is defined between two surfaces that are allowed to separate and slide across each other but are not allowed to penetrate. Variations of the sliding interface, such as tied interfaces, tied-sliding (tension-compression) and rigid walls, are available as well. As of version 1.2 it is also possible to model the fluid flow across two contacting biphasic materials. Finally, the user may specify a body force to model the effects such as, gravity, base acceleration or centripetal acceleration.

FEBio has a large library of element formulations. These include linear and quadratic tetrahedral, hexahedral and pentahedral (wedge) elements. FEBio also supports triangular quadrilateral shell elements, with linear and quadratic interpolations.

FEBio is a nonlinear implicit FE solver and does not have mesh generation capabilities. The finite element mesh, as well as all constitutive parameters and loading is defined in an input file, the format of which is described in detail in this document. This input file needs to be generated by preprocessing software. The preferred preprocessor for FEBio is called *FEBioStudio*. FEBioStudio can convert some other formats to the FEBio input specification. For instance, NIKE3D [43] and Abaqus input files can be imported in FEBioStudio and can be exported from as a FEBio input file.

1.2 About this document

This document is part of a set of three manuals that accompany FEBio: the User's Manual, describing how to use FEBio (this manual), a Developer's Manual for users who wish to modify or add features to the code, and a *FEBio Theory Manual*, which describes the theory behind the FEBio algorithms.

This document discusses how to use FEBio and describes the input file format in detail. Chapter 2 describes how to run FEBio and explains the various command line options. It also discusses the different files that are required and created by FEBio. Chapter 3 describes the format of the FEBio input file. An XML-based format is used, organizing the data in a convenient hierarchical structure. Chapter 4 gives a detailed overview of the available constitutive models. Chapter 5 discusses the restart capabilities of FEBio. The restart feature allows the user to interrupt a run and continue it at a later time, optionally making changes to the problem data. Chapter 5.6.2 describes the multi-step analysis feature, which allows the user to split up the entire analysis into several steps. Chapter 6 explains how to setup and run a parameter optimization problem using FEBio's optimization module. Chapter 7 provides helpful information for troubleshooting an FEBio model and offers guidelines that help users avoid common problems.

Although this document describes some of the theoretical aspects of FEBio, a complete theoretical development can be found in the *FEBio Theory Manual*. Developers who are interested in

modifying or extending the FEBio code will find the *FEBio Developer's Manual*[1] very useful.

1.3 FEBio Basics

This section provides a brief overview of how FEBio works. For more details regarding the algorithms in FEBio, please consult the FEBio Theory Manual.

When FEBio starts, first it will load the configuration file, where it will find instructions on what linear solver to use, what plugins to load, etc. Please see section 8 for more information regarding the configuration file.

Usually FEBio will read the input file that was specified on the command line next. The input file contains all the information that FEBio needs to build the FE Model and solve it. At the very least the input file will define the mesh, the materials, boundary conditions, time stepping, and analysis parameters. This document describes the structure of the FEBio input file in detail. See 3and 4.

Next, FEBio will start solving the model defined by the input file and proceed as follows:

1. **Loop over all analysis steps**. A model can define multiple analysis steps. In each step the boundary conditions, time stepping, and analysis parameters can be modified (e.g. a two-step analysis where a model is loaded statically in the first step. In the second step the load is released and the dynamic response is sought.)

2. **For each analysis step, loop over all time steps**: In each analysis step, loads are usually applied incrementally for stability reasons over a period of time. The time parameter can represent the actual physical time (e.g. in dynamic simulations), or a pseudo-time (e.g. quasi-static loading of an elastic model.). For more on time stepping see 3.3.

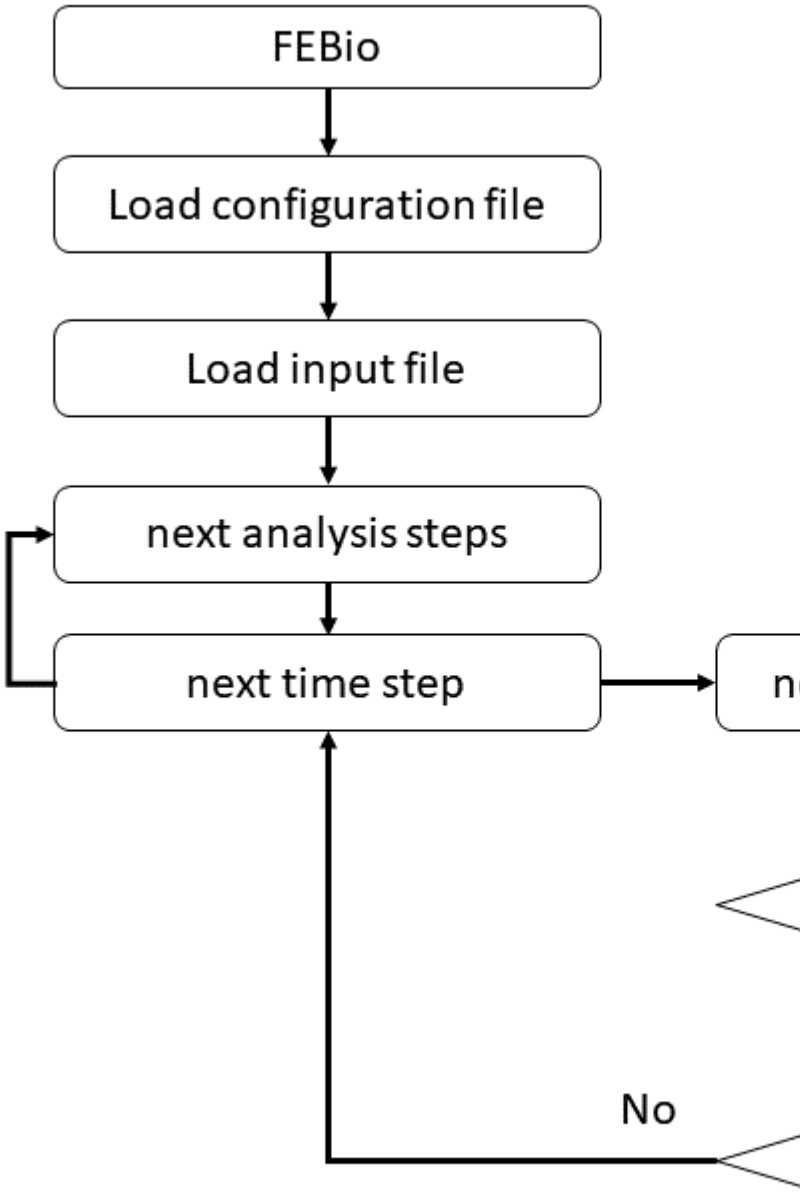
3. **Solve each time step**: for each time step FEBio will solve the corresponding finite element equations. Usually they are nonlinear and thus are solved with a nonlinear solution strategy. In FEBio this is a variation of the Newton method. See section 3.3for more information.

4. **Check convergence**: Since Newton's method is an iterative method convergence is determined by comparing the norms of the solution and residual to the user-defined values in the input file. What norms are used will depend on the physics of the problem, as well as on several user control parameters. See 3.3.

5. **Augmentation**: In models that define some type of constraint (e.g. contact, rigid joints, etc.), FEBio will do an additional calculation after a time step converges, called an augmentation. This is because FEBio does not calculate the exact Lagrange multiplier that enforce the constraints, but instead uses an iterative algorithm (called augmented Lagrangian method) to approximate the Lagrange multipliers. During the augmentation, FEBio updates the approximate Lagrange multipliers. If the updates to the multipliers are small, FEBio will terminate the time step, otherwise it will restart the time step with the updated multipliers.

See the figure below for an overview of the basic FEBio flow.

[1] The developers manual is only available online (see `http://febio.org` for more information)



1.4 Units in FEBio

FEBio does not assume a specific unit system. It is up to the user to enter numbers that are defined in consistent units. For example, when entering material parameters in SI units, the user must enter all loads, contact parameters, and other boundary conditions in SI units as well. The units of all the parameters are given when they are defined in this manual. We use a generic

designation of units for all the parameters using the following symbols.

Symbol	***Name***	***SI unit***
L	Length	meter (m)
M	Mass	kilogram (kg)
t	Time	second (s)
T	Temperature	Kelvin (K)
n	Amount of substance	mole (mol)
F	Force	Newton (kg·m/s^2)
P	Pressure, stress	Pascal (Pa=N/m^2)
Q	Electric charge	Coulomb (C=A·s)

Units are given using the bracket notation. For instance, the unit for density is [**M**/**L**^{3}] and the unit for permeability is [**L**^{4}/**F**·**t**]. When using SI units, this corresponds to units of kg/m^3 for density and m^4/N.s for permeability, respectively. Unitless parameters are designated by empty brackets (**[ ]**). The units for angles are either [**deg**] for degrees or [**rad**] for radians.

When adopting a consistent set of units, first choose a primary set of units, and then determine the remaining derived units. For example, in typical problems in solid mechanics, the primary set consists of three units. If you choose [**M**]=kg, [**L**]=m, and [**t**]=s, then [**F**]=N and [**P**]=Pa. Alternatively, if you choose [**L**]=mm, [**F**]=N and [**T**]=s as the primary set, then [**P**]=MPa (since 1 N/mm^2 = 10^{6}N/m^2 = 1 MPa) and [**M**]=tonne (tonne = N ·s^2/mm). The primary set of units must be independent. For instance, in the last example, you cannot choose [**P**] as a primary unit as it can be expressed in terms of [**F**] and [**L**] (i.e. [**P**]=[**F**/**L**^{2}]).

Example:

Primary Units	
time	s
length	mm
force	N
amount of substance	nmol
charge	C
temperature	K
Derived Units	
stress	N/mm^2, MPa
permeability	mm^4/N·s, mm^2/Pa·s
diffusivity	mm^2/s
concentration	nmol/mm^3, mM
charge density	nEq/mm^3, mEq/L
voltage	mV
current density	A/mm^2
current	A

Chapter 2

Running FEBio

FEBio is a command line application which means it does not have its own Graphical User Interface (GUI) and must be run from a shell or command line. FEBio runs on several different computing platforms including Windows, Mac OSX and many versions of Linux. The command line input and output options are described in this chapter.

2.1 Running FEBio on Windows

There are several ways to run FEBio on Windows. The easiest way is by simply selecting the FEBio program from the Programs menu or by double-clicking the FEBio icon in the installation folder. However, this runs FEBio with the installation folder as the working folder, and unless the FEBio input files are in this folder, you will need to know the relative or absolute path to your input files. A more practical approach is to run FEBio from a command prompt. Before you can do this, you need to know two things: how to open a command prompt and how to add the FEBio installation folder to your PATH environment variable so that you can run FEBio from any folder on your system[1]. The process is slightly different depending on whether you are using Windows XP or Windows 7, so we'll look at the two Windows versions separately.

2.1.1 Windows XP

First, we'll add the FEBio installation folder to the PATH variable. Open the *Control Panel* from the *Start* menu. Switch to *Classic View* and double-click the *System* icon. In the dialog box that appears, select the *Advanced* tab and click the button named *Environment variables*. Find the *path* variable and click the *Edit* button. At the end of the PATH's value (don't delete the current value) type a semi-colon and then the absolute path to the FEBio installation folder (e.g. C:/Program Files/FEBio/). Then click the *OK*-button on all open dialog boxes.

To open a command prompt, click the *Run* menu item on the *Start* menu. In the dialog box that appears type *cmd* and press the *OK*-button. A command prompt window appears. You can now use the *cd* (change directory) command to navigate to the folder that contains the FEBio input files. To run FEBio, simply type *febio* (with or without additional arguments) and press *Enter*.

[1] The current FEBio installers should automatically setup the environment path so that FEBio can be run from anywhere on the file system.

2.1.2 Windows 7

Let's first modify the *PATH* environment variable. Open the *Start* menu and type *system* in the search field. From the search results, select the *System* option under *Control Panel*. The *System* window will appear. Find the *Change Settings* option (on the lower, right side) and click it. The System Properties dialog box appears. Activate the *Advanced* tab and click the *Environment Variables* button. Find the *path* variable and click the *Edit* button. At the end of the PATH's value (don't delete the current value) type a semi-colon and then the absolute path to the FEBio installation folder (e.g. C:/Program Files/FEBio/). Then click the *OK*-button on all open dialog boxes.

Next, open a command prompt as follows. Click the *Start* menu and type *cmd* in the search field. From the search results, select the *cmd* option under Programs. A command prompt window appears. You can now use the *cd* (change directory) command to navigate to the folder that contains the FEBio input files. To run FEBio, simply type *febio* (with or without additional arguments) and press *Enter*.

2.1.3 Running FEBio from Explorer

A third method of running FEBio, which often is very convenient, is to run FEBio from Windows Explorer. To do this, first open Explorer and browse to the folder that contains your FEBio input files. Next, right-click on the input file and select *Open With*. Now select *Choose default program*. A dialog box appears with a list of programs to open the input file. If FEBio is not on this list yet, click the *Browse* button. Locate the FEBio executable (e.g. in C:/Program Files/FEBio2/bin), select it and press the *Open* button. Now select FEBio in the *Open With* dialog box and press Ok.

After you have done this once, the process simplifies. After you right-click the input file, FEBio should now show up in the *Open With* menu item and can be selected immediately without having to go through all the previous steps.

2.2 Running FEBio on Linux or MAC

Running FEBio on Linux or Mac is as easy as opening up a shell window and typing FEBio on the command line. However, you may need to define an alias to the folder that contains the FEBio executable if you want to run FEBio from any folder on your system. Since this depends on your shell, you need to consult your Linux documentation on how to do this. E.g. if you are using c-shell, you can define an alias as follows:

```
alias febio '/path/to/febio/executable/'
```

If you don't want to define this alias every time you open a shell window, you can place it in your shell start up file (e.g. *.cshrc* for c-shell).

2.3 The Command Line

FEBio is started from a shell window (or the *command prompt* in Windows). The command line is the same for all platforms:

```
febio [-o1 [name1] | -o2 [name2] | ... ]
```

Where -o1, -o2 are options and *name1*, *name2*, ... are filenames. The different options (of which most are optional) are given by the following list:

-i name of input file

-r restart file name

-g debug flag

-p plot file name

-o log file name

-c data check only

-s material parameter optimization control file

-d diagnostic input file

-dump Set restart option and optional dump file name

-nosplash don't show the welcome screen

-config configuration filename

-noconfig don't use the configuration file

-break set a break point

-import load a plugin

A more detailed description of these options follows.

-i The -i option is used to specify the name of the input file. The input file is expected to follow the format specifications as described in Chapter 3.

Example:

```
> febio -i input.feb
```

This is the most common way to start a FEBio run. However, FEBio allows the omission of the -i when only a filename is given.

```
> febio input.feb
```

On Windows, this allows for starting FEBio by double-clicking on an input file (assuming you have chosen FEBio as the default program to open .feb files). Note that if additional options are specified on the command line the -i must be present.

-r The -r option allows you to restart a previous analysis. The filename that must follow this option is a FEBio *restart input file* or a *dump file*. The restart input file and dump file are described in more detail in 2.8.3. The -i and -r options are mutually exclusive; only one of them may appear on the command line.

Example:

```
> febio -r file.feb
```

-g The –g option runs FEBio in *debug mode*. See Section 2.8.2 for more information on running FEBio in debug mode.

Example:

```
> febio -i input.feb -g
```

-p The –p option allows the user to specify the name of the *plot file*. The plot file is a binary file that contains the main results of the analysis. FEBio usually provides a default name for this file; however, the user can override the default name using this option. See Section 2.7 for more details on the output files generated by FEBio.

Example:

```
> febio -i input.feb -p out.plt
```

-o The –o option allows the user to set the name of the *log file*. The log file will contain a record of the screen output that was generated during a run. FEBio usually provides a default name for this file (see Section 2.7), but the user can override it with this command line option.

Example:

```
> febio -i input.feb -o out.log
```

-c When the –c option is specified on the command line, FEBio will only read the input file and check it for possible errors. When the check is complete, FEBio will terminate. See Section 2.8.4 for more details on this option.

Example:

```
> febio -i input.feb -c
```

-nosplash When the –nosplash command is entered on the command line, FEBio will not print the welcome message to the screen. This is useful when calling FEBio from another application and when the user wishes to suppress any screen output from FEBio. Other options for suppressing output can be set in the control section of the FEBio input file (see Section 3.3.1).

Example:

```
> febio -i input.feb -nosplash
```

-silent When the –silence option is specified on the command line, FEBio will not generate any output to the screen. Unless explicitly instructed not to, FEBio will still create a log file which will have the convergence information.

Example:

```
> febio -i input.feb -silent
```

-config

-noconfig As of version 1.2, FEBio uses a *configuration file* to store platform specific settings. Usually FEBio assumes that the location for this configuration file is the same as the executable. However, the user can specify a different location and filename using the –config command line option. If the user does not have a configuration file or does not wish to use one, this can be specified using the –noconfig option. More details on the configuration file can be found in Section 2.5 and Chapter 8.

Example:

```
> febio -i input.feb -cnf C:\path\to\febio.xml.
```

-s This option instructs FEBio to run a material parameter optimization on the specified input file. The optimization module is described in detail in Chapter 6. The –s option is followed by the optimization control file which contains among other things the parameters that need to be optimized. Note that the restart feature does not work with the optimization module.

Example:

```
> febio -i file.feb -s control.feb
```

-d This option will run a FEBio diagnostics. A diagnostic is a special type of test that can be used to verify an implementation. For example, the *tangent diagnostic* allows users to check the consistency between the material's stress and tangent implementations.

Example:

```
> febio -d diagnostic.feb
```

-dump It is possible to restart a previous run using the restart capability in FEBio. This is useful when a run terminates unexpectedly. If that happens, the user can restart the analysis from the last converged timestep. Before this feature can be used, the user must request the creation of a *dump file*. This file will store all the information that FEBio will need to restart the analysis. FEBio will usually provide a default name for the dump file, but the *–dump* command line option allows the user to override the default name for the dump file. See Section 2.8.3 and Chapter 5 for more details on how to use the restart feature.

Example:

```
> febio -i input.feb -dump out.dmp
```

-break With this option a break point can be set which sets a time point at which FEBio will interrupt the run and show the FEBio prompt. The following example sets a break point at time 1.0. FEBio will interrupt the run after the time step at time 1.0 is reached (i.e. has converged).

Example:

```
> febio -i file.feb -break 1.0
```

-import This command will load the plugin that is specified following this command line option. Although it is more convienient to list plugins in the FEBio configuration file, this option allows users to load a plugin from the command line, if such a need would arise.

Example:

```
> febio -import myplugin.dll
```

2.4 The FEBio Prompt

At the FEBio prompt allows users to manipulate the currently active model or further configure FEBio. The FEBio prompt is shown when you start FEBio without any command arguments, or when a run is interrupted either by the user (using ctrl+c) or by reaching a breakpoint. The FEBio prompt will look something like this:

```
febio>
```

You can now enter one of the following commands:

break Add a breakpoint, which will stop FEBio at a particular time point or event. A breakpoint can be defined at a particular (simulation) time or at an event. To define a breakpoint at a particular time, just enter the time value after the break command. To break at an event, specify the event name at which to pause the run. The following list of events are defined.

Event	Description
ALWAYS	break on any event
INIT	break after model initialization
STEP_ACTIVE	break after step activation
MAJOR_ITERS	break after major iteration (i.e. time step) converged
MINOR_ITERS	break after minor iteration (i.e. Newton iteration)
SOLVED	break after the model is solved
UPDATE_TIME	break before time is incremented
AUGMENT	break before augmentation
STEP_SOLVED	break after step is solved
MATRIX_REFORM	break after global matrix is reformed

breaks Prints list of current breakpoints.

clear Clear one or all breakpoints.

config Load (or reload) a configuration file.

cont Continue an interrupted run. FEBio will continue the analysis where it left off.

conv force the current time step to converge. This is useful for example when a time step is having difficulty satisfying too tight of convergence criteria. The user can then manually force the convergence of the time step. However, if the convergence difficulties are due to instabilities, forcing a time step to converge could cause the solution to become unstable or even incorrect. Also be aware that even if the solution recovers on later timesteps, the manually converged step might be incorrect.

debug Entering *debug* will toggle debug mode. Adding *on* (*off*) will turn the debug mode on (resp. off). In debug mode, FEBio will store additional information to the log and plot file that could be useful in debugging the run. It is important to note that since FEBio will store all non-converged states to the plot file, this file may become very large in a short number of time steps. See Section 2.8.2 for more details on debugging.

fail Stop the current iteration and retry. If the current time step is not converging and if the auto-time stepper is enabled, the fail command will stop the current time step and retry it with a smaller time step size. If the auto-time stepper is not enabled, the fail command will simply exit the application.

help Prints an overview of available commands with a brief description of each command.

load load a plugin file

out Write the current linear system (matrix and right hand side vector) to a file.

plot Write the current state of the model to the plot database. This command is useful when you want to store the non-converged state at the current iteration. Note that this command only stores the state at the current iteration. If you turn on debug mode, all the iterations are stored to the plot file.

plugins Print a list of the plugins that are loaded.

print Print the value of variables. The following variables can be printed.

nnz Number of nonzeroes in global stiffness matrix.

time The simulation time.

neq Number of equations.

quit Stop the current model, or exit FEBio if no model is running.

restart Toggles the restart flag. When the restart flag is set, FEBio will create a dump file at the end of each converged time step. This dump file can then later be used to restart the analysis from the last converged time step. See Section 2.8.3 and Chapter 5 for more details on FEBio's restart feature.

run run an FEBio input file. This command takes the same options as you can enter on the command line. For example, to run a file named *test.feb* from the FEBio prompt, type the following:

```
run -i test.feb
```

svg Write the sparse matrix profile to an svg file.

time Print progress time statistics.

unload unload a plugin from FEBio

version Print version information.

You can also bring up the FEBio prompt during a run by pressing ctrl+c[2]. See Section 2.8.1 for more details.

[2]This feature does not work on some Linux platforms and may abruptly terminate the run.

2.5 The Configuration File

As of version 1.2, FEBio uses a *configuration file* to store platform-specific settings, such as the default linear solver and the list of plugins that need to be loaded at startup. The configuration file uses an xml format to store data and is detailed in Chapter 8. For backward compatibility, it is still possible to run FEBio without the configuration file. In that case, the default settings prior to version 1.2 are used.

Example:

```
> febio -i myfile.feb -noconfig
```

The default configuration file needs to be stored in the same location as the executable and named *febio.xml*. Alternatively, the location and the name of the file can also be specified on the command line using the –cnf option.

Example:

```
> febio -i myfile.feb -config /home/my/folder/FEBio/febio.xml
```

2.6 Using Multiple Processors

As of version 2.0, FEBio uses OpenMP to parallellize several of the finite element calculations, improving the performance considerably. Both the right-hand-side and the stiffness matrix evaluations for many types of problems have been parallelized. On a system with four processors, a speedup of 2-3 can be expected, depending on the size and type of model. Models with complex material behavior (such as EFD-type materials, biphasic, multiphasic materials, etc.) will benefit most from these parallelization efforts. In addition, FEBio implements the *MKL* version of the *PARDISO* linear solver, which is a parallel linear solver using OpenMP.

To use multiple processors set the environment variable OMP_NUM_THREADS to the number of desired threads. You should set the number of threads to be equal or less than the number of processors on your system (Setting it higher may actually decrease performance). For example, on a system with four processors you can set the environment as follows. On Linux using the Bash shell, execute:

```
> export OMP_NUM_THREADS=4
```

Using the c-shell, execute:

```
> setenv OMP_NUM_THREADS 4
```

Or at a Windows command prompt:

```
> set OMP_NUM_THREADS=4
```

On Windows, you can add this environment variable as well from the Control Panel. On Win7, open the Control Panel (*Start→Control Panel*). Open the System panel and click *Change Settings*. The *System Properties* dialog box should open up. Select the *Advanced Tab* and click the *Environment Variables* button. In the next dialog box, click the *New...* button under the *User variables*. Enter OMP_NUM_THREADS for the variable name and 4. Click OK on all open dialog boxes.

A note on repeatability When using multiple processors, it can not always be guaranteed that all calculations are executed in the same order and, due to numerical round-off, the results of these calculations will not always be the same. In FEBio, this means that the same model run repeatedly on the same machine with multiple processors, may give slightly different convergence norms or even slightly different answers. In many cases, the differences should be small, but in some problems that are prone to ill-conditioning (e.g. contact) the discrepancies may be more significant. When running on one processor, the results of consecutive runs should always be identical.

2.7 FEBio Output

2.7.1 Screen output

By default, FEBio will print convergence and progress information to the screen that informs users how the analysis is progressing. The output depends on the particular module and solver that was chosen in the FEBio input file, as well as some user-defined settings, but in general provides the following information.

- **Time stepping information**: The current time step that FEBio is solving and a notification when the time step completed (or an error message why the time step failed to complete)
- **Convergence information**: for each time step, FEBio usually has to solve a nonlinear problem for which an iterative nonlinear solver is used. Several "norms" are printed to inform the user how FEBio is progressing toward the solution of the nonlinear problem.
- **Summary:** At the end of the analysis a summary is printed with heuristics that inform the user how well the model ran.

By default, all screen output will also be printed to the log flie.

2.7.2 Output files

After running FEBio, two or three files are created: the *log file*, the *plot file* and optionally the *dump file*. The log file is a text file that contains the same output (and usually more) that was written to the screen. The *plot file* contains the results of the analysis. Since this is a binary file, the results must be analyzed using post processing software such as *PostView*. In some cases, the user may wish to request the creation of a *dump file*. This file contains temporary results of the run. If an analysis terminates unexpectedly or with an error, this file can be used to restart the analysis from the last converged time step. See Section 2.8.3 and Chapter 5 for more details. The names of these files can be specified with the command options –p (plot file), -a (dump file), -o (log file). If one or more of the file names following these flags are omitted, then the omitted file name(s) will be given a default name. The default file names are derived from the input file name. For example, if the input file name is *input.feb* the logfile will have the name *input.log*, the plot file is called *input.xplt* and the dump file is called *input.dmp*.

Note 1. The name of the log and plot file can also be specified in the FEBio input file. See Section 3.16 for more information.

Note 2. When running an optimization problem the name of the log file is derived from the optimization control file. See Chapter 6 for more information on running optimization problems with FEBio.

2.8 Advanced Options

2.8.1 Interrupting a Run[3]

The user can pause the run by pressing ctrl+c. This will bring up the FEBio prompt, and the user can enter a command. The FEBio prompt will also be shown when FEBio reaches a break point. See Section 2.4 for a list of available commands. Note that it may take a while before the FEBio prompt is displayed after the user requests a ctrl+c interruption. This may be because the program is in the middle of a call to the linear solver or another time-consuming part of the analysis procedure that cannot be interrupted.

2.8.2 Debugging a Run

As stated in Section 2.3, FEBio can be run in debug-mode by specifying the –g option on the command line. When running in debug mode, FEBio performs additional checks and prints out more information to the screen and to the plot file. It will also store all non-converged states to the plot file. These non-converged states can be very useful for determining the cause of non-convergence or slow convergence. Because of this additional work, the problem may run slightly slower. Note that debug mode can be turned on/off while running an analysis by first interrupting the run with ctrl+c and then using the *debug* command to toggle the debug mode on or off. It is important to note that since FEBio will store all non-converged states to the plot file, this file may become very large in a short number of time steps. An alternative approach is to use the *plot* command to write out select non-converged states.

2.8.3 Restarting a Run

When the creation of a restart dump file is requested, the analysis can be restarted from the last converged timestep. This is useful when the run terminated unexpectedly or when the user wishes to modify some parameters during the analysis. To request the creation of a dump file, simply add the -dump flag on the command line. This will generate a *dump* file which then can be used to restart the analysis. You can specify an optional dump level, which sets how often the dump file is created, and an optional dump file name.

```
> febio -i input.feb -dump
```

With the optional arguments, the complete syntax would be:

```
>febio -i input.feb -dump=1 out.dmp
```

The dump level can set to 1 (= write dump file after each converged time step), or 2 (= write dump file after each completed step).

To restart an analysis, use the -r command line option. This option requires a filename as a parameter, and this name can be either the name of a dump file or the name of a restart input file. The latter case is a text file that allows the user to redefine some parameters when restarting the run. The format of this file is described in Chapter 5.

[3] This feature may not work properly on all systems, although it will always work on Windows systems.

2.8.4 Input File Checking

The $-c$ option allows the user to stop FEBio after the initial data checking is done. This way, potential input errors can be spotted without running the actual problem.

Example:

```
> febio -i input.feb -c
```

Chapter 3

Free Format Input

This chapter describes the XML-based input format used by FEBio. Since this format follows standard XML conventions, the files can be viewed with any file viewer that supports XML files. Since the free format input file is a text file, it can be edited with any text editor.

An XML file is composed of a hierarchical list of *elements*. The first element is called the *root element*. Elements can have multiple *child elements*. All elements are enclosed by two *tags:* a tag defining the element and an *end tag*. A simple example of an XML file might look like this:

```
<root>
  <child>
    <subchild> ... </subchild>
  </child>
</root>
```

The *value* of an element is enclosed between the name and the end tag.

```
<element> here is the value </element>
```

Note that the XML format is case-sensitive.

XML elements can also have *attributes* in name/value pairs. The attribute value must always be quoted using quotation marks (") or apostrophes (')[1].

```
<element attr="value">...</element>
<element attr='value'>...</element>
```

If an XML element has no value, an abbreviated syntax can be used. The following two lines are identical.

```
<element [attribute list]></element>
```

or

```
<element [attribute list]/>
```

Comments can be added as follows.

[1] Support for apostrophes was not added until FEBio version 2.1.

```
<!-- This is a comment -->
```

The first line in the document – the XML declaration – defines the XML version and the character encoding used in the document. An example can be:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
```

3.1 Free Format Overview

The free format organizes the FEBio input data into hierarchical XML elements. The root element is called *febio_spec*. This root element also defines the format version number (Note that FEBio and the input format specification follow different version numberings). This document describes version 3.0 of the FEBio specification[2] (see Section 3.1.1 below for more details on the different input specification formats). The root element will therefore be defined as follows:

```
<febio_spec version="3.0">
<!-- contents of file -->
</febio_spec>
```

The different sections introduced in this chapter are child elements of this root element. The following sections are currently defined:

Module defines the physics module for solving the model.

Control specifies control and solver parameters.

Globals Defines the global variables in the model

Material Specifies the materials used in the problem and the material parameters.

Mesh Defines the mesh of the problem, including nodal coordinates and element connectivity.

MeshDomains Assigns materials and other formulation attributes to element sets.

MeshData Defines element, facet, edge or nodal data that can be mapped to material parameters or certain boundary conditions and loads.

Initial Defines initial conditions for dynamic problems, such as initial velocities, and for transient quasi-static problems.

Boundary Defines the boundary conditions that are applied on the geometry.

Loads Defines the loads applied to the model. This includes nodal loads, boundary loads and volume loads (or sources for heat transfer problems).

Contact This section defines all contact interfaces.

Constraints This section defines rigid and nonlinear constraints.

Discrete This section defines all the discrete elements (i.e. springs)

[2] FEBio continues to read some older formats, but they are considered to be obsolete.

LoadData Defines the load controllers.

Ouput Defines additional data that is to be stored.

Step Defines different analysis steps, where in each analysis the boundary, loads, contact and initial conditions can be redefined.

The current format specification expects the different sections of the input file to be listed in the same order as given above. Not all sections are required. Empty sections can be omitted and some are optional. A minimal file must contain at least the Control, Material, Mesh, and MeshDomains sections. The rest of this chapter describes each of these sections in more detail.

3.1.1 Format Specification Versions

This document describes version 3.0 of the FEBio input specification. This format differs in several aspects from the previous versions of the input specification. This section describes the major changes between the different versions.

- **Version 3.0**: The latest and recommended version of the FEBio input specification described in this document. The major focus of this revision was adding support for FEBio 3.0's features for modeling heterogeneous parameters. Heterogeneous parameters can be created via mathematical expressions or via the MeshData section. It also introduces a more consistent way for referencing model parameters. The *Geometry* section was replaced with the *Mesh* and *MeshDomains* sections in order to further separate the definition of the mesh and its physical attributes (e.g. material assignments).
- **Version 2.5**: This format differs from its predecessor in some important aspects: all nodesets, surfaces, etc., that are used by boundary conditions, loads, contact, etc., must be defined in the Geometry section. Boundary conditions, loads, contact, etc., are now defined by referencing the sets in the Geometry section. This format also adds the *MeshData* section and reformats the *Discrete* section. Rigid node sets and prescribed rigid degrees of freedom are moved to the *Boundary* section. This format is **still supported** but considered obsolete.
- **Version 2.0**: This is the first major revision of the input file format and redefines many of the file sections: The *Elements* section uses a different organization. Elements are now grouped by material and element type. Multiple *Elements* sections can now be defined to create multiple parts. Surfaces can now be defined in the *Geometry* section and referenced by boundary conditions and contact definitions. A new *Contact* section contains all the contact definitions. A new *Discrete* section was defined that contains all the materials and definitions of the discrete elements (e.g. springs). The *Boundary* section is also redesigned. This format is **still supported** but considered obsolete.
- **Version 1.3**: This was an experimental version that redefined the *Geometry* section, but was later abandoned in favor of version 2.0. This version is **no longer supported**.
- **Version 1.2**: A *Loads* section was added and all surface and body loads are now defined in this section instead of the *Boundary* section. This version is **mostly supported** but considered obsolete.
- **Version 1.1**: Rigid body constraints are no longer defined in the rigid material definition but instead placed in a new *Constraints* section. This version is **no longer supported**.

- **Version 1.0**: The original input format specification. This version is **no longer supported**.

As of FEBio 3.0, only versions 1.2, 2.0, 2.5 are supported. Versions 1.2 and 2.0 are considered obsolete and it is highly recommended to convert older files to the new 3.0 specification for use with newer versions of FEBio. This can be done for instance using FEBioStudio.

3.1.2 Notes on backward compatibility

Some features that were available in versions prior to 3.0 are no longer supported or require a different syntax.

1. The *Parameters* section is no longer supported. This section allowed users to define file parameters that could be used as parameter values. This section was removed since it was difficult to support in FEBio Studio and a better mechanism was implemented for defining model-level parameters. (See the *Globals* section.)

2. Some fiber materials defined the *theta* and *phi* parameters for setting the fiber orientation. These parameters are no longer supported. Instead, the fiber direction should be specified via the *fiber* property, or if the *fiber* property is not available, the *mat_axis* property.

```
<fiber type="angles">
  <theta>90</theta>
  <phi>0</phi>
</fiber>
```

3.1.3 Multiple Input Files

FEBio supports distributing the model definition across multiple input files. This can greatly facilitate defining large, complex models and allows the re-use of model input files without the need to create the entire model input file from scratch. When using multiple input files to define a model, you must create a control input file that may reference other input files. This control file will be used to run the model in FEBio. There are two ways of including a file into the control file: The *Include* section, and the *from* attribute.

3.1.3.1 Include Keyword

The *Include* keyword[3] can be used to include the contents of another FEBio input file. The filename is entered as the value of the tag.

```
<Include>example.feb</Include>
```

The included file must be a valid FEBio file in that it must begin with the *febio_spec* tag and contain sections defined in this document. However, the included file does not need to define a complete model definition. For instance, it can contain only the *Mesh* section.

Note that the contents of the entire file will be included. This is different from the *from* attribute discussed below, which can be used to include only certain sections from files.

[3] Supported from FEBio version 2.3 and up.

3.1.3.2 The 'from' Attribute

The *from* attribute can be used to include sections from other files. All the main sections defined in Section 3.1 support the *from* attribute which can be used to load the section from another input file. For example, to load the *Material* section from the file mat.feb, defining the *Material* section in the control input file as follows.

```
<Material from="mat.feb"/>
```

FEBio will now read the *Material* section from this child file. The child file must be a valid FEBio input file, meaning it must begin with the *febio_spec* root section, but does not have to be complete. For example, the file mat.feb only needs to define the Material section. However, the child file may contain other sections. In that case, only the section referenced in the control file will be read from the child file. For example, if the file *in.feb* contains both the *Material* and the *Mesh* section, the control file can read both these sections as follows.

```
<Material from="in.feb"/>
<Mesh from="in.feb"/>
```

To give a more concrete example, assume that the *Material*, *Mesh*, and *Boundary* sections are defined in the files *mat.feb*, *geom.feb*, and *bc.feb* respectively. The control input file could then look like the following.

```
<febio_spec version="3.0">
  <Control>
    <time_steps>10</time_steps>
    <step_size>0.1</step_size>
  </Control>
  <Material from="mat.feb"/>
  <Mesh from="geom.feb"/>
  <Boundary from="bc.feb"/>
</febio_spec>
```

Notice that the *Control* section is still defined in the control file. The control file can contain a combination of explicit section definitions and referenced sections using the *from* attribute. As mentioned above, the control file is used to run the model in FEBio. So, if the control file is called *model.feb* then the model is run as follows.

```
>febio -i model.feb
```

When FEBio parses the control file it will automatically parse the referenced child files it encounters in the control input file.

3.2 Module Section

The module section defines the type of analysis to perform with FEBio. This section must be defined as the first section in the input file. It takes on the following format:

```
<Module type="[type]"/>
```

where *type* can be any of the following values:

type	Description
solid	Structural mechanics analysis: quasi-static or dynamic
biphasic	Biphasic analysis: steady-state or transient
solute	Biphasic analysis including solute transport: steady-state or transient
multiphasic	Multiphasic analysis including solute transport and chemical reactions
heat	Heat transfer analysis: steady-state or transient (1)
fluid	Fluid mechanics analysis: steady-state or dynamic
fluid-FSI	Fluid mechanics with fluid-structure interactions: steady-state or dynamic

For example:

```
<febio_spec version="3.0">
  <Module type="solid"/>
  <!-- rest of file -->
</febio_spec>
```

Comments:

1. The heat module requires a plugin.

Notes:

1. In version 1.2 the Module section was optional. If omitted it was assumed that the *solid* module was used. In version 2.0 the Module section is required and must be the first section in the file.
2. Older versions of FEBio (format specification 1.2 and before) allowed you to run a poroelastic (now called biphasic) problem by simply defining a poroelastic material. This is no longer possible. You need to define the proper Module section to run a biphasic analysis. If you have a file that no longer works as of version 1.4 of FEBio, you'll need to insert the following Module section in the file as the first section of the file.

```
<febio_spec version="3.0">
  <Module type="biphasic"/>
  <!-- rest of the file unaltered -->
</febio_spec>
```

3.3 Control Section

The control section is defined by the *Control* element. This section defines all parameters that are used to control the evolution of the solution as well as parameters for the nonlinear solution procedure. These parameters are defined as child elements of the *Control* element and depend somewhat on the analysis as defined by the *Module* section. The control section defines the control parameters, the solver parameters, and optionally, the time_stepper parameters.

Example:

```
<Control>
    <analysis>STATIC</analysis>
    <time_steps>50</time_steps>
    <step_size>0.02</step_size>
    <solver>
        <max_refs>25</max_refs>
        <max_ups>0</max_ups>
        <diverge_reform>1</diverge_reform>
        <reform_each_time_step>1</reform_each_time_step>
        <dtol>0.001</dtol>
        <etol>0.01</etol>
        <rtol>0</rtol>
        <lstol>0.9</lstol>
        <min_residual>1e-20</min_residual>
        <qnmethod>BFGS</qnmethod>
        <rhoi>-2</rhoi>
    </solver>
    <time_stepper>
        <dtmin>0.0002</dtmin>
        <dtmax>0.02</dtmax>
        <max_retries>5</max_retries>
        <opt_iter>6</opt_iter>
    </time_stepper>
</Control>
```

3.3.1 Control Parameters

The following parameters are common for all analysis. If not specified they are assigned default values, which are found in the last column. An asterisk (*) after the name indicates a required parameter. The numbers behind the description refer to the comments following the table.

Parameter	Description	Default
analysis	Sets the analysis type (1)	static
time_steps*	Total number of time steps. (= *ntime*)(2)	(none)
step_size*	The initial time step size. (= *dt*) (2)	(none)
plot_level	Sets the level of state dumps to the plot file (3)	PLOT_MAJOR_ITRS

plot_range	Set the range of the states that will be stored to the plot file (4)	0,-1
plot_stride	Set the stride of the states that will be stored to the plot file (4)	1
plot_zero_state	Flag that controls whether the "zero" state will be written to the plot file, even if it is not defined in the range (4)	0 (false)
print_level	Sets the amount of output that is generated on screen (5)	PRINT_MINOR_ITRS
output_level	Controls when to output data to file (6)	OUTPUT_MAJOR_ITRS
integration	Set the integration rule for a particular element (7)	N/A

Comments:

1. The *analysis* element sets the analysis type. Currently, FEBio defines three analysis types: (quasi-)static, steady-state, and dynamic. In a quasi-static analysis, inertial effects are ignored and an equilibrium solution is sought. Note that in this analysis mode it is still possible to simulate time dependant effects such as viscoelasticity. In a dynamic analysis the inertial effects are included.

Value	**Description**
static	(quasi-) static analysis
steady-state	steady-state response of a transient (quasi-static) biphasic, biphasic-solute, multiphasic, fluid or fluid-FSI analysis
dynamic	dynamic analysis for solid, fluid and fluid-FSI analyses

2. The total running time of the analysis is determined by *ntime* * *dt*. Note that when the auto-time stepper is enabled (see below), the actual number of time steps and time step size may be different than specified in the input file. However, the total running time will always be determined by *ntime* * *dt.*

3. The *plot_level* allows the user to control exactly when the solution is to be saved to the plot file. The following values are allowed:

Value	**Description**
PLOT_NEVER	Don't save the solution
PLOT_MAJOR_ITRS	Save the solution after each converged timestep
PLOT_MINOR_ITRS	Save the solution for every quasi-Newton iteration
PLOT_MUST_POINTS	Only save the solution at the must points

The PLOT_MUST_POINTS option must be used in conjunction of a *must-point* curve. See the comments on the *dtmax* parameter for more information on must-point curves. When the *plot_level* option is set to PLOT_MUST_POINTS, only the time-points defined in the must-point curve are stored to the plotfile.

4. When using the fixed time stepper, several parameters control which time steps are stored to the plot file.

   The *plot_range* parameter sets the range of the states that will be stored to the plot file. The range is defined by two values that specify the first and last time step that will be stored to the plot file. The value "0" refers to the initial time step, usually time zero, and negative values count backwards from the final time step (as defined by the *time_steps* parameter). For instance, the default values,

   ```
   <plot_range>0,-1</plot_range>
   ```

   store all time steps to the plot file, including the initial "zero" time step. As another example, to store only the last five time steps, set

   ```
   <plot_range>-5,-1</plot_range>
   ```

   By default, all time steps within the range will be stored to the plot file. Time steps can be skipped using the *plot_stride* parameter. For instance, to store only every 10 steps, set

   ```
   <plot_stride>10</plot_stride>
   ```

   Note that the first and last time step defined by the range will always be stored, regardless of the plot stride.

   The "zero" time step refers to the initial state of the model, before any calculations are done. This state will only be stored to the plot file if the minimal value of the plot range is set to zero. To force storing this state to the plot file, set the *plot_zero_state* parameter to one.

   ```
   <plot_zero_state>1</plot_zero_state>
   ```

   This will store the zero time step to the plot file, even when it is not specified inside the plot range.

   Again, the *plot_range*, *plot_stride*, and *plot_zero_state* parameters are only used by the fixed time stepper. Currently, these parameters are not used with the auto time stepper.

5. The *print_level* allows the user to control exactly how much output is written to the screen. The following values are allowed:

Value	**Description**
PRINT_NEVER	Don't generate any output
PRINT_PROGRESS	Only print a progress bar
PRINT_MAJOR_ITRS	Only print the converged solution
PRINT_MINOR_ITRS	Print convergence information during equilibrium iterations
PRINT_MINOR_ITRS_EXP	Print additional convergence info during equilib. iterations

6. The *output_level* can be used to control when FEBio outputs the data files. The following values are supported.

Value	Description
OUTPUT_NEVER	Don't generate any output
OUTPUT_MUST_POINTS	Only output at must points
PRINT_MAJOR_ITRS	Output at end of each time step
PRINT_MINOR_ITRS	Output at each iteration
OUTPUT_FINAL	Only output the data at the last converged time step.

7. You can override FEBio's default integration rule for specific element classes. For each element class, define a *rule* element in which you set the integration rule.

```
<integration>
  <rule elem="<elem>">VALUE</rule>
  <!-- repeat rules for other elements -->
</integration>
```

The *elem* attribute value defines for which element class you wish to override the default integration rule and can have any of the following values.

elem	Description
hex8	8-node hexahedral element
hex20	20-node quadratic hexahedral element
tet4	4-node linear tetrahedral element
tet10	10-node quadratic tetrahedral element
tet15	15-node quadratic tetrahedral element
penta15	15-node quadratic pentahedral element
tri3	3-node linear triangles (e.g. for contact)
tri6	6-node quadratic triangles

The values of the rule elements depend on the *elem* attribute. The tables below show the available integration rules for the different element types. The values marked with an asterisk (*) are the default.

- For the *hex8* element, the following values are defined.

hex8	Description
GAUSS8*	Gaussian integration using 2x2x2 integration points.
POINT6	Alternative integration rule for bricks using 6 integration point

- For the *hex20* element, the following values are defined.

hex20	Description
GAUSS8	Gaussian integration using 2x2x2 integration points.
GAUSS27*	Gaussian integration using 3x3x3 integration points.

- For the *tet4* element, the following values are allowed.

tet4	Description
GAUSS4	Gaussian integration rule using 4 integration points.
GAUSS1*	Gaussian integration rule using one integration point.
UT4	Nodally integrated tetrahedron. (1)

Comments:

1. The UT4 is a special formulation for tetrahedral elements that uses a nodally averaged integration rule, as proposed by Gee et al [29]. This formulation requires additional parameters. To override the default values, use the following alternative syntax:

```
<rule elem="tet4" type="UT4">
  <alpha>0.05</alpha>
  <iso_stab>0</iso_stab>
</rule>
```

The *alpha* parameter defines the amount of "blending" between the regular tet-contribution and the nodally integrated contribution. The value must be between 0 and 1, where 0 means no contribution from the regular tet and 1 means no contribution from the nodally averaged tet. The *iso_stab* parameter is a flag that chooses between two slightly different formulations of the nodally integrated tet. When set to 0, the stabilization is applied to the entire virtual work, whereas when set to 1 the stabilization is applied only to the isochoric part. See the *FEBio Theory Manual* for a detailed description of this formulation.

- For the *tet10* element, the following integration rules are supported.

tet10	description
GAUSS4*	Gaussian integration rule using 4 integration points
GAUSS8	Gaussian integration rule using 8 integration points
LOBATTO11	Gauss-Lobatto integration rule using 11 integration points

Notes:

The Lobatto integration rule differs from a regular Gauss integration rule in that it includes the vertices of the tetrahedral element. The *Lobatto11* integration rule uses the 10 tetrahedral nodes, plus one integration rule located at the center of the element.

- For the *tet15* element, the following integration rules are defined.

tet15	description
GAUSS8	Gaussian integration rule using 8 integration points
GAUSS11	Gaussian integration rule using 11 integration points
GAUSS15	Gaussian integration rule using 15 integration points

- For the *penta15* element, the following values are defined.

penta15	Description
GAUSS8	Gaussian integration using 2x2x2 integration points.
GAUSS21*	Gaussian integration using 3x7 integration points.

- For the *tri3* element, the following integration rules are supported.

tri3	description
GAUSS1	Gaussian integration with one integration point
GAUSS3*	Guassian integration with three integration rules.

- For the *tri6* element, the following integration rules are supported.

tri6	description
GAUSS3*	Gaussian integration with 3 integration points
GAUSS6	Gaussian integration with 6 integration points
GAUSS4	Gaussian integration with 4 integration points
GAUSS7	Gaussian integration with 7 integration points
LOBATTO7	Gauss-Lobatto integration with 7 integration points.

Notes:

The GAUSS6 rule has only nonzero weights at the edge nodes, which effectively reduces this rule to a 3-node rule.

3.3.2 Time Stepper parameters

The optional *time_stepper* element sets the parameters that control the FEBio auto-time stepper. This auto-time stepper will adjust the time step size depending on the convergence stats of the previous time step. It defines the following parameters.

Value	Description	Default
dtmin	Minimum time step size (1)	
dtmax	Maximum time step size (3)	
opt_iter	Optimal, or desired, number of iterations per time step (2)	10
max_retries	Maximum number of times a time step is restarted. (2)	5
aggressiveness	Algorithm for cutting the time step size after a failed time step	0

Comments:

1. The *dtmin* and *dtmax* values are used to constrain the range of possible time step values. The *opt_iter* defines the estimated optimal number of quasi-Newton iterations. If the actual number of iterations is less than or equal to this value the time step size is increased, otherwise it is decreased.

2. When a time step fails (e.g. due to a negative jacobian), FEBio will retry the time step with a smaller time step size. The *max_retries* parameter determines the maximum number of times a timestep may be retried before FEBio error terminates. The new time step size is determined by the ratio of the previous time step size and the *max_retries* parameter. For example, if the last time step size is 0.1 and *max_retries* is set to 5, then the time step size is adjusted by 0.02: The first retry will have a step size of 0.08; the next will be 0.06, and so on.

3. The user can specify a load curve for the *dtmax* parameter. This load curve is referred to as the *must-point* curve and serves two purposes. Firstly, it defines the value of the *dtmax* parameter as a function of time. This can be useful, for instance, to enforce smaller time steps during rapid loading or larger time steps when approaching steady-state in a transient analysis. Secondly, the time points of the *dtmax* loadcurve define so-called *must-points*. A must-point is a time point where FEBio must pass through. This is useful for synchronizing the auto-time stepper with the loading scenario. For instance, when loading starts at time 0.5, adding a must-point at this time will guarantee that the timestepper evaluates the model at that time. In conjunction with the PLOT_MUST_POINT value of the *plot_level* parameter, this option can also be used to only write results to the plotfile at the specified time points. Consider the following example.

```
<dtmax lc="1">0.1</dtmax>
...
<loadcurve id="1" type="step">
  <loadpoint>0,0</loadpoint>
  <loadpoint>0.5, 0.1</loadpoint>
  <loadpoint>1.0, 0.2</loadpoint>
</loadcurve>
```

This example defines load curve 1 as the *must-point* curve. This curve defines three points where FEBio will pass through (namely 0, 0.5 and 1.0). The values of each time point is the value of the maximum time-step size (*dtmax*). Since the curve is defined as a step-function, each value is valid up to the corresponding time-point. Thus, between time 0 and time 0.5, the maximum time step value is 0.1. Between 0.5 and 1.0 the maximum time step value is 0.2. If the *plot_level* parameter is set to PLOT_MUST_POINTS, then only the three defined time points will be stored to the plotfile.

3.3.3 Common Solver Parameters

Many of the solvers define the same parameters. They are listed in the table below. Additional parameters that are only defined for a specific type of analysis are listed in the following sections.

Parameter	Description	Default
etol	Convergence tolerance on energy (1)	0.01
rtol	Convergence tolerance on residual (1)	0 (disabled)
lstol	Convergence tolerance on line search (2)	0.9
lsmin	minimum line search step	0.01
lsiter	Maximum number of line search iterations	5
max_refs	Max number of stiffness reformations (3)	15
qnmethod	Quasi-Newton update method (3)	0 (BFGS)
max_ups	Max number of BFGS/Broyden stiffness updates (3)	10
cmax	Set the max condition number for the stiffness matrix (4)	1e+5
diverge_reform	Flag for reforming stiffness matrix when the solution diverges (3)	1

min_residual	Sets minimal value for residual tolerance (6)	1e-20
symmetric_stiffness	Use symmetric stiffness matrix flag (7)	1
equation_scheme	Set the equation allocation scheme	0
equation_order	Set the equation allocation ordering	0
optimize_bw	Optimize bandwidth of stiffness matrix (5)	0

Comments:

1. FEBio determines convergence of a time step based on three convergence criteria: displacement, residual and energy (that is, residual multiplied by displacement). Each of these criteria requires a tolerance value that will determine convergence when the relative change will drop below this value. For example, a displacement tolerance of ε means that the ratio of the displacement increment (i.e. the solution of the linearized FE equations, $\Delta\mathbf{U} = -\mathbf{K}_k^{-1}\mathbf{R}_k$) norm at the current iteration $k+1$ to the norm of the total displacement ($\mathbf{U}_{k+1} = \mathbf{U}_k + \Delta\mathbf{U}$) must be less than ε:
$$\frac{\|\Delta\mathbf{U}\|}{\|\mathbf{U}_{k+1}\|} < \varepsilon$$
For the residual and energy norms, it is the ratio of the current residual norm (resp. energy norm) to the initial one that needs to be less than the specified convergence tolerance.

   To disable a specific convergence criterion, set the corresponding tolerance to zero. For example, by default, the residual tolerance is zero, so that this convergence criterion is not used.

2. The *lstol* parameter controls the scaling of the vector direction obtained from the line search. A line search method is used to improve the convergence of the nonlinear (quasi-) Newton solution algorithm. After each BFGS or Newton iteration, this algorithm searches in the direction of the displacement increment for a solution that has less energy (that is, residual multiplied with the displacement increment) than the previous iteration. In many problems this will automatically be the case. However, in some problems that are very nonlinear (e.g. contact), the line search can improve convergence significantly. The line search can be disabled by setting the *lstol* parameter to zero, although this is not recommended.

3. The *qnmethod* parameter determines the quasi-Newton update method. For the BFGS method set *qnmethod* to 0 (default); for Broyden's method set *qnmethod* to 1. The *max_ups* and *max_refs* parameters control the BFGS/Broyden method that FEBio uses to solve the nonlinear FE equations. In this method the global stiffness matrix is only calculated at the beginning of each time step. For each iteration, a matrix update is then done. The maximum number of such updates is set with *max_ups*. When FEBio reaches this number, or if the solution diverges and *diverge_reform* is set to 1, it reforms the global stiffness matrix (that is, it recalculates it) and factorizes it, essentially taking a "full Newton" iteration. Then FEBio continues with BFGS/Broyden iterations. The *max_refs* parameter is used to set the maximum of such reformations FEBio can do, before it fails the timestep. In that case, FEBio will either terminate or, if the auto-time stepper is enabled, retry with a smaller time step size.

   Note that when max_ups is set to 0, FEBio will use the Full-Newton method instead of the BFGS method. In other words, the stiffness matrix is reformed for every iteration. In this

case it is recommended to increase the number of *max_refs* (to e.g. 50), since the default value might cause FEBio to terminate prematurely when convergence is slow.

4. When the condition number of the stiffness matrix becomes too large, inversions of the stiffness matrix become inaccurate. This will negatively affect the convergence of the quasi-Newton or Newton solution algorithm. FEBio monitors the condition number of the BFGS stiffness update and when it exceeds *cmax* it reforms the stiffness matrix.

```
<cmax>1e5</cmax>
```

5. The *optimize_bw* parameter enables bandwidth minimization for the global stiffness matrix. This can drastically decrease the memory requirements and running times when using the skyline solver. It is highly recommended when using the skyline solver.

```
<optimize_bw>1</optimize_bw>
```

   When using a different linear solver (e.g., pardiso or SuperLU), the bandwidth optimization can still be performed if so desired. However, for these solvers there will be little or no effect since these solvers are not as sensitive to the bandwidth as the skyline solver.

6. If no force is acting on the model, then convergence might be problematic due to numerical noise in the calculations. For example, this can happen in a displacement driven contact problem where one of the contacting bodies is moved before initial contact is made. When this happens, the residual norm will be very small. When it drops below the tolerance set by *min_residual*, FEBio will assume that there is no force acting on the system and will converge the time step.

7. The *symmetric_stiffness* flag is used to set the symmetry of the global stiffness matrix. Only specify this flag if you want to override the default symmetry, which depends somewhat on the analysis type. Forcing a symmetric matrix when the problem is non-symmetric may have negative impact on convergence. The values for this parameter are:
   - 0 = unsymmetic
   - 1 = symmetric
   - 2 = structurally symmetric

3.3.4 Solver Parameters for a Structural Mechanics Analysis

A structural mechanics analysis is defined by using the *solid* type in Module section. The solver parameters are given in the table below:

Parameter	Description	Default
dtol	convergence tolerance on displacement	0.001

3.3.5 Solver Parameters for Biphasic Analysis

A biphasic analysis is defined by using the *biphasic* type in Module section. Since a biphasic analysis couples a fluid problem to a solid mechanics problem, all control parameters above can be used in a biphasic analysis. In addition, the following parameters can be defined:

Parameter	Description	Default
ptol	Specify the fluid pressure convergence tolerance	0.01

3.3.6 Solver Parameters for Solute and Multiphasic Analyses

When the type attribute of the Module section is set to *solute* or *multiphasic*, an analysis is solved that includes solute transport. All parameters for a biphasic analysis can be used (including the ones for a structural mechanics analysis). In addition, the following parameters can be specified:

Parameter	Description	Default
ctol	Specify the concentration convergence tolerance	0.01

3.3.7 Solver Parameters for Heat Analysis

A heat analysis uses the parameters defined in Section 3.3.1. However, not all parameters have an effect. In particular, any parameter related to the auto-time stepping capability of FEBio or the nonlinear solution strategy is ignored.

3.3.8 Solver Parameters for Fluid and Fluid-FSI Analyses

A fluid analysis is defined by using the *fluid* type in Module section (see Section 3.2). In addition to the common parameters, the following parameters can be specified:

Parameter	Description	Default
vtol	convergence tolerance on velocity	0.001
ftol	convergence tolerance on dilatation	0.001
rhoi	Spectral radius parameter ρ_∞	0
reform_each_time_step	Flag for reforming stiffness matrix at the start of each time step	1

A fluid-structure interaction analysis is defined by using the *fluid-FSI* type in Module section. It uses the parameters of *solid* and *fluid* analyses.

Transient fluid and fluid-FSI analyses may often run very efficiently using Broyden's method (*qnmethod* set to 1) with *max_ups* set to 50; efficiency may be further increased by setting *reform_each_time_step* to 0, which will postpone reforming the stiffness matrix at subsequent time steps until *max_ups* updates have been exhausted. When using Broyden's method with fluid and fluid-FSI analyses, set *rtol* to a non-zero value to ensure an accurate solution, for example *rtol*=0.001 (see Section 3.3.1).

The spectral radius parameter ρ_∞ determines the time integration scheme: Values in the range $0 \leq \rho_\infty \leq 1$ use the generalized $\alpha-$method (see *FEBio Theory Manual*). With $\rho_\infty = 0$, damping of higher frequency components (such as those produced by a step increase in velocity) occurs theoretically within a single time step; in contrast, with $\rho_\infty = 1$, no damping occurs, potentially leading to instability in the solution process. When solving transient flows that exhibit eddies or shed vorticies, a value of $\rho_\infty = 0.5$ represents a good balance between too much and too little numerical damping.

3.4 Globals Section

The *Globals* section is used to define some global variables, such as global constants, solute data and solid bound molecule data.

3.4.1 Constants

Global constants currently include the universal gas constant R [**F**·**L**/**n**·**T**], absolute temperature θ [**T**], and Faraday constant F_c [**Q**/**n**]. These constants must be expressed in units consistent with the rest of the analysis:

```
<Globals>
  <Constants>
    <R>8.314e-6</R>
    <T>298</T>
    <Fc>96485e-9</Fc>
  </Constants>
</Globals>
```

3.4.2 Solutes

In biphasic-solute, triphasic and multiphasic analyses, a unique identifier must be associated with each solute in order to enforce consistent nodal degrees of freedom across boundaries of different materials. This unique identification is achieved by listing each solute species that appears in the entire finite element model and associating it with a unique *id*, *name*, and providing its charge number z^α, molar mass M^α, and density ρ_T^α:

```
<Globals>
  <Solutes>
    <solute id="1" name="Na">
      <charge_number>1</charge_number>
      <molar_mass>22.99</molar_mass>
      <density>0.97<density>
    </solute>
    <solute id="2" name="Cl">
      <charge_number>-1</charge_number>
      <molar_mass>35.45</molar_mass>
      <density>3.21<density>
    </solute>
    <solute id="3" name="Glc">
      <charge_number>0</charge_number>
      <molar_mass>180.16</molar_mass>
      <density>1.54<density>
    </solute>
  </Solutes>
</Globals>
```

These solute identification numbers should be referenced in the *sol* attribute of solutes when defining a biphasic-solute (Section 4.8.2), triphasic or multiphasic material (Section 4.9.2).

The molar mass and density of solutes are needed only when solutes are involved in chemical reactions. When not specified, default values for these properties are set to 1.

3.4.3 Solid-Bound Molecules

In multiphasic analyses with chemical reactions involving solid-bound molecules, a unique identifier must be associated with each such molecule in order to enforce consistent properties across the entire model. This unique identification is achieved by listing each solid-bound species that appears in the entire finite element model and associating it with a unique *id*, *name,* charge number, molar mass and density:

```
<Globals>
  <SolidBoundMolecules>
    <solid_bound id="1" name="CS">
      <charge_number>-2</charge_number>
      <molar_mass>463.37</molar_mass>
      <density>1.5<density>
    </solid_bound >
  </SolidBoundMolecules >
</Globals>
```

The *id* number should be referenced in the *sbm* attribute of solid-bound molecules when included in the definition of a multiphasic material (Section 4.9). The charge number is used in the calculation of the fixed charge density contributed by this solid-bound molecule to the overall solid matrix fixed-charge density. The density is used in the calculation of the contribution of this molecule to the referential solid volume fraction. The density and molar mass are used in the calculation of the molar volume of this molecule in chemical reactions.

3.5 Material Section

The material section is defined by the *Material* element. This section defines all the materials and material parameters that are used in the model. A material is defined by the *material* child element. This element has two attributes: *id,* which specifies a number that is used to reference the material, and *type*, which specifies the type of the material. The *material* element can also have a third optional attribute called *name*, which can be used to identify the material by a text description. A material definition might look like this:

```
<material id="1" type="isotropic elastic">
```

Or, if the optional *name* attribute is present:

```
<material id="2" type="rigid body" name="femur">
```

The material parameters that have to be entered depend on the material type. A complete list of available materials is provided in Chapter 4.

3.6 Mesh Section

The *Mesh* section contains all the mesh data, including nodal coordinates and element connectivity. It has the following sub-sections:

Nodes defines the nodal coordinates of the mesh

Elements defines the elements of the mesh

NodeSet defines a node set

Edge defines an edge, i.e. a set of line elements

Surface defines a surface, i.e. a set of facets

DiscreteSet defines a set of discrete elements (e.g. springs)

ElementSet defines an element set

SurfacePair define a surface pair that can be used by a contact definition.

At least one *Nodes* must be defined and one *Elements* section. The other sections are optional. The *NodeSet*, *Edge*, *Surface*, *DiscreteSet*, *ElementSet*, and *SurfacePair* sections define sets of nodes, edges, facets, discrete elements, elements, and surface pairs, respectively, and can be referenced by other sections of the model file. For instsance, boundary conditions can be defined by referencing the sets to which the boundary condition will be applied.

3.6.1 Nodes Section

The *Nodes* section contains nodal coordinates. It has an optional attribute called *name*. If this attribute is defined, the *Nodes* section also defines a node set.

```
<Nodes [name="<set name>"]>
```

The nodes are defined using the *node* tag which is a child of the *Nodes* section. Repeat the following XML-element for each node:

```
<node id="n">x,y,z</node>
```

The *id* attribute is the global identifier of the node and must be a unique number within the model definition. This *id* is used as a reference in the element connectivity section.

Multiple *Nodes* sections can be defined, but each node can only be defined once. For example:

```
<Nodes name="set01">
  <node id="1">0,0,0,</node>
  ...
  </node id="101">1,1,1</node>
</Nodes>
<Nodes name ="set02">
  <node id="102">2,1,1</node>
  ...
  <node id="999">2,2,2</node>
</Nodes>
```

3.6.2 Elements Section

The *Elements* sections contain a list of the element connectivity data. Multiple *Elements* sections can be defined. The *Elements* section has the following attributes.

Attribute	Description
type	element type
name	unique name that identifies this domain

Each *Elements* section contains multiple *elem* elements that define the element connectivities. Each *elem* tag has a *id* attribute that defines the element number. For example, the following *Elements* section defines a list of hexahedral elements:

```
<Elements type="hex8" name="part1">
  <elem id="1">1,2,3,4,5,6,7,8</elem>
  <elem id="2">1,2,3,4,5,6,7,8</elem>
  <...>
</Elements>
```

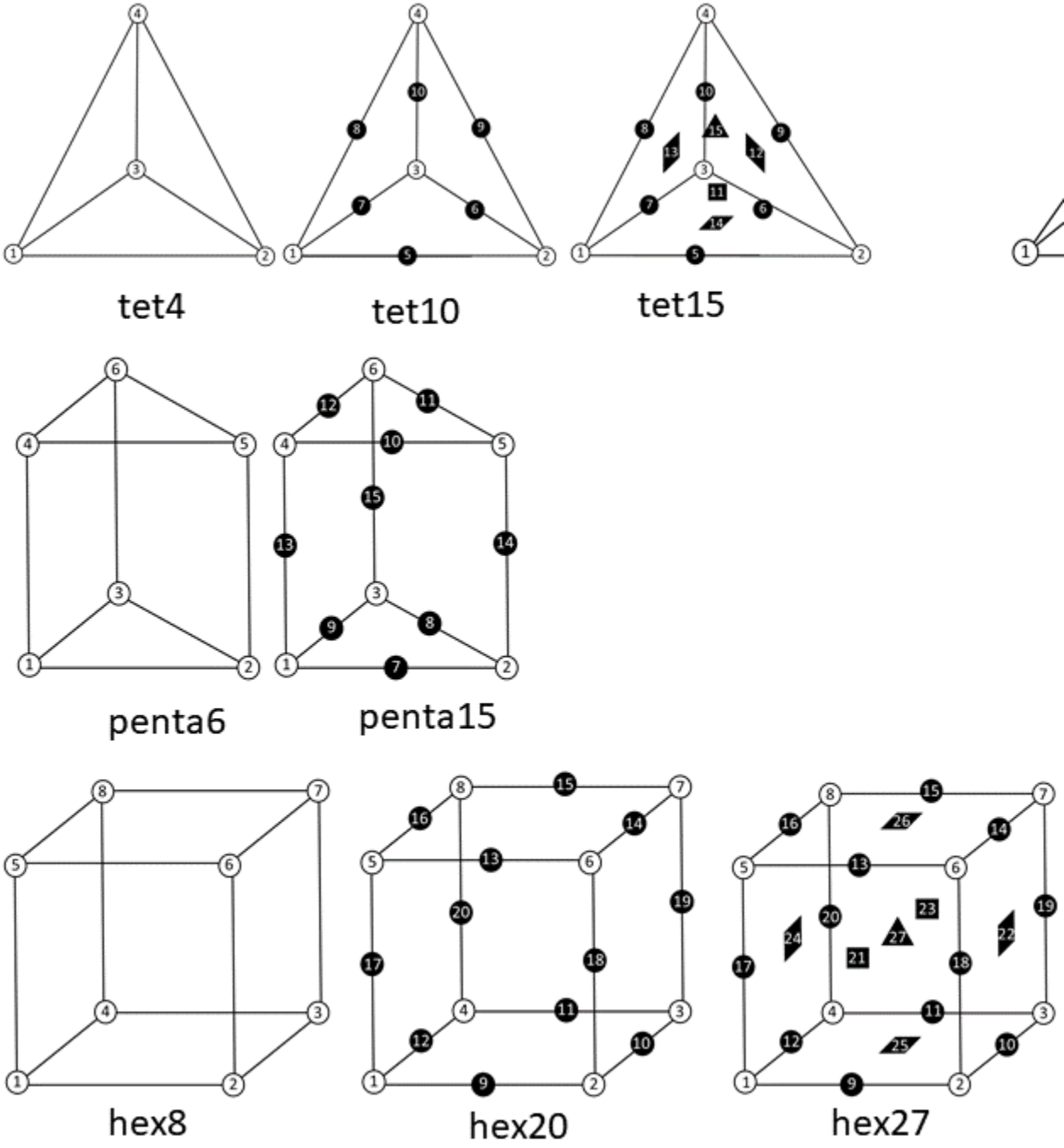
FEBio classifies elements in two categories, namely *solids* and *shells*.

3.6.2.1 Solid Elements

The following solid element types are defined:

hex8	8-node trilinear hexahedral element
hex20	20-node quadratic hexahedral elements
hex27	27-node quadratic hexahedral elements
penta6	6-node linear pentahedral (wedge) element
penta15	15-node quadratic pentahedral (wedge) element
pyra5	5-node linear pyramidal element
tet4	4-node linear tetrahedral element
tet10	10-node quadratic tetrahedral element
tet15	15-node quadratic tetrahedral element

The node numbering has to be defined as in the figure below.



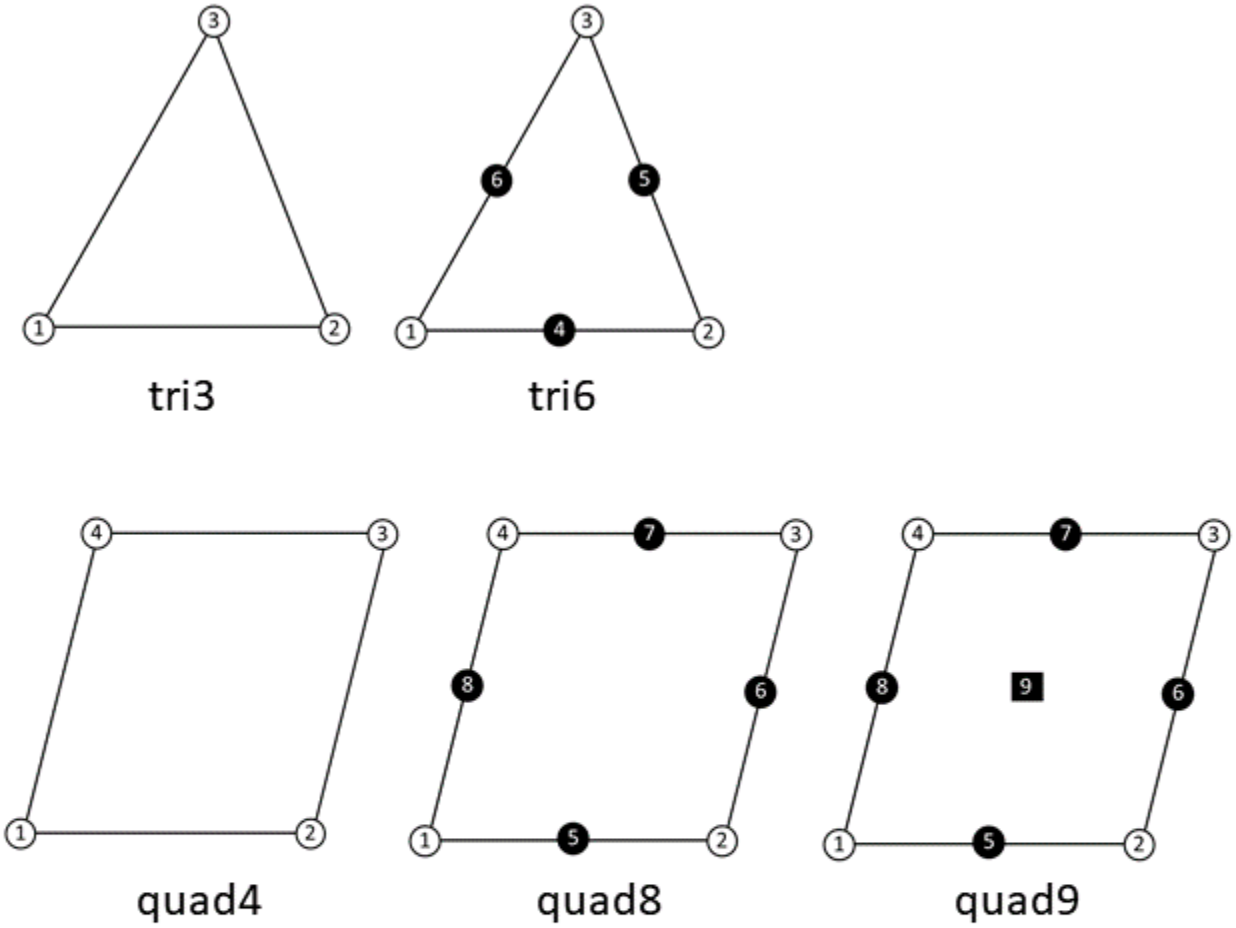
Node numbering for solid elements

3.6.2.2 Shell Elements

FEBio currently supports the following shell elements:

tri3	3-node linear triangular shell element (compatible strain)
tri6	6-node quadratic triangular shell element (compatible strain)
quad4	4-node linear quadrilateral shell element (compatible strain)
quad8	8-node quadratic quadrilateral shell element (compatible strain)
quad9	9-node quadratic quadrilateral shell element (compatible strain)
q4ans	4-node linear quadrilateral shell element (assumed natural strain)
q4eas	4-node linear quadrilateral shell element (enhanced assumed strain)

For shell elements that use a *compatible strain* formulation, the calculation of strain components is based on nodal displacements, similar to hexahedral or pentrahedral elements. Users should be aware that this compatible strain formulation is very susceptible to element locking when the shell thickness is much smaller than the shell size (e.g., when the aspect ratio is less than 0.01). Therefore, these shell formulations should be used with caution, keeping in mind this important constraint. Conversely, these shell elements perform very well when they are attached to solid elements (e.g., skin over muscle), or sandwiched between shell elements (e.g., cell membrane separating cytoplasm from extra-cellular matrix), as described in [34].



Node numbering for shell elements

The element-locking limitation of compatible strain shell formulations has motivated the development of specialized shell formulations that attempt to overcome locking. The FE literature on this subject is rather extensive and we refer the reader to the excellent review chapter by Bischoff et al. [17] on this topic. Methods for overcoming locking include the assumed natural strain (ANS) formulation for transverse shear strains [42, 14] and transverse normal strains [15, 16]. The ANS

formulation may be supplemented with the enhanced assumed strain (EAS) method [52] and extended to large deformations [36, 56, 50]. FEBio includes the ANS (*q4ans*) and EAS (*q4eas*) quadrilateral shell element formulations of Vu-Quoc and Tan [56], using a seven-parameter EAS interpolation, which is otherwise substantially similar to the five-parameter interpolation presented in an earlier study by Klinkel et al. [36]. These shell elements are not suitable for attachment to a solid element, nor sandwiching between two solid elements. Since they don't experience element locking, they should be loaded more slowly than compatible strain shell elements. The most accurate of these shell formulation is *q4eas*.

By default, the nodes of a shell element define its *front* face. The location of the shell element *back* face is calculated from the nodal values of the shell thickness, along the opposite direction of nodal normals. The nodal normal is evaluated by averaging the front face normal of all shell elements sharing that node. When a shell element is attached to a solid element (e.g., when the shell nodes also represent the nodes of one face of the solid element), FEBio automatically accounts for the shell thickness, reducing the height of the solid element in the direction of the shell normal. It is the user's responsibility to ensure that the shell thickness is less than that of the solid element; otherwise, a negative Jacobian error will be automatically generated.

Prior to FEBio 2.6, the nodes of a shell element defined its *middle* face (halfway between front and back, such that the shell element extends above and below the face defined by the shell nodes). This older formulation can be recovered by setting *shell_formulation* to 0 in the *Control* section. This setting only works with compatible strain shell formulations.

When shell domains intersect such that three or more shell elements share the same edge, as in a T-connection, users should set *shell_normal_nodal* to 0 in the *Control* section. This setting ensures that the back face of a shell element is calculated using the front face normal, instead of nodal normals, since the latter would be ill-defined for nodes belonging to such an edge.

Finally, please note that shell elements cannot be stacked in FEBio.

3.6.3 NodeSet Section

The *NodeSet* section allows users to define node sets. These node sets can then later be used in the definition of the fixed and prescribed boundary conditions. A node set is defined by the *NodeSet* tag. This tag takes one required attribute, *name*, which defines the name of the node set. A node set definition is followed by a list of nodes. For each a *node* tag is defined which requires one attribute, named "id", which takes the node number as its value. For example,

```
<NodeSet name="nodeset1">
  <node id="1"/>
  <node id="2"/>
  <node id="101"/>
  <node id="102"/>
</NodeSet>
```

Node sets can also be nested.

```
<NodeSet name="set1"> ... </NodeSet>
<NodeSet name="set2"> ... </NodeSet>
<NodeSet name="set3">
  <NodeSet node_set="set1"/>
  <NodeSet node_set="set2"/>
<NodeSet>
```

This is useful for defining larger nodesets without repeating node numbers.

3.6.4 Edge Section

The *Edge* section allows users to define a set of edges. These edges can be used to define boundary conditions or load.s

```
<Edge name="edge1">
  <line2 lid="1">1,2</line2>
  <line2 lid="2">2,3</line2>
</Edge>
```

Here, the *lid* attribute defines the *local* id of the edge, local with respect to the edge definition. The local ids must begin at 1 and defined sequentially.

The edge elements are defined by using a tag that depends on the type of the edge element. The following edge elements are currently supported.

line2 2-node line element

line3 3-node line element

3.6.5 Surface Section

The *Surface* section allows users to define surfaces. These surfaces can then later be used to define the boundary conditions and contact definitions. A surface definition is followed by a list of surface elements, following the format described below.

```
<Surface name="named_surface">
  <quad4 lid="1">1,2,3,4</quad4>
  <...>
</Surface>
```

The *Surface* takes one required attribute, namely the *name*. This attribute sets the name of the surface. This name will be used later to refer back to this surface.

The following surface elements are available:

quad4 4-node quadrilateral element

quad8 8-node serendipity quadrilater element

tri3 3-node triangular element

tri6 6-node quadratic triangular element

tri7 7-node quadratic triangular element

The value for the surface element is the nodal connectivity:

```
<quad4 id="n">n1,n2,n3,n4</quad4>
<tri3 id="n">n1,n2,n3</tri3>
```

Surface elements cannot overlap element boundaries. That is, the surface element must belong to a specific element. Surface elements do not contribute to the total number of elements in the mesh. They are also not to be confused with shell elements.

3.6.6 ElementSet Section

The *ElementSet* section can be used to define an element set. Element sets can be used to output data for only a subset of elements. An element set is defined through the *ElementSet* tag, which takes one attribute, namely *name* that specifies the name of the element set. For each element in the set, an *elem* tag is defined which takes the element id as an attribute. For example,

```
<ElementSet name="set01">
  <elem id="1001"/>
  <elem id="1002"/>
  <elem id="1003"/>
</ElementSet>
```

3.6.7 DiscreteSet Section

The *DiscreteSet* section defines sets of discrete elements. These sets can then be used to define e.g. springs.

```
<DiscreteSet name="springs">
  <delem>1,2</delem>
  <delem>3,4</delem>
</DiscreteSet>
```

3.6.8 SurfacePair Section

The *SurfacePair* section defines a pair of surfaces that can be used to define surface-to-surface interactions (e.g. contact).

```
<SurfacePair name="contact1">
  <primary surface="surface1"/>
  <secondary surface="surface2"/>
</SurfacePair>
```

The surfaces (i.e. *surface1* and *surface2*) are surfaces defined in the *Surface* section. Because surfaces must already be defined before they can be referenced in the *SurfacePair* section, the *Surface* must be defined before the *SurfacePair* section.

3.7 MeshDomains Section

The *MeshDomains* section assigns various physical attributes to the element sets of the mesh. For each of the *Elements* sections in the *Mesh* section, define a *SolidDomain* or a *ShellDomain* section, depending on whether the elements are solid or shells. Each domain also requires a material name that defines the material properties of the domain.

3.7.1 SolidDomain Section

Use the *SolidDomain* section to define a solid domain. This section takes two parameters:

name The name of the element set (defined via an *Elements* section). This element set must only contain solid elements.

mat The name of the material that will be assigned to this domain

3.7.2 ShellDomain Section

Use the *ShellDomain* section to define a shell domain. This section takes two parameters:

name The name of the element set (defined via an *Elements* section). This element set must only contain shell elements.

mat The name of the material that will be assigned to this domain

3.8 MeshData Section

The *MeshData* section is where data is specified that can be mapped to the mesh. The data can be applied to a parameter of the model, e.g. a material parameter, or a pressure load.

To define a mesh data section add one of the following tags.

NodeData Define data on a node set

SurfaceData Define data on a surface

ElementData Define data on an element set

The following attributes can be added.

name All mesh data require a name, which can be specified with the *name* attribute. This name will be used by model parameters to reference the particular mesh data.

datatype defines the type of data

The following table lists the supported data types.

data type	Description
scalar	A single floating point value
vec2	A 2D vector defined as x, y
vec3	A 3D vector defined as x, y, z

If the data type is not defined, the *scalar* data type is assumed.

node_set/surface/elem_set Specifies the set for which to define the data.

There are two mechanisms to define mesh data: The values can be tabulated, which is detailed below, or can be generated via data generators, which is described in the next section. To use a data generator, specify the *generator* attribute.

3.8.1 Data Generators

The *generator* attribute is optional, but can be defined if the user wishes to generate the data automatically instead of tabulating it. If the generator attribute is defined, the child tags must be the parameters of the generator. For example

```
<MeshData>
  <node_data name="E_map" generator="math">
    <math>X*X + Y*Y + Z*Z</math>
  <mesh_data>
</MeshData>
```

The following generators are currently suppored.

const The *const* generator takes a constant value and assigns it to the set.

```
<MeshData>
  <mesh_data name="rotation" type="mat3" generator="const" elem_set="Part1">
    <value>1,0,0, 0,1,0, 0,0,1</value>
  <mesh_data>
</MeshData>
```

math The *math* generator generates the data based on a mathematical expression.

```
<MeshData>
  <mesh_data name="fiber" type="vec3" generator="math" elem_set="Part1">
    <math>X,Y,Z</math>
  <mesh_data>
</MeshData>
```

Note that in math expressions, only the variables X, Y, and Z can be used, which refer to reference coordinates.

parabolic_map The "*parabolic map*" defines a scalar data field with a parabolic profile on a surface. The data is determined by solving a heat-type problem with a constant source and homogeneous boundary conditions on the edge of the surface.

```
<MeshData>
  <mesh_data name="pressure" generator="parabolic map" surface="surface1">
    <value>1.0</value>
  <mesh_data>
</MeshData>
```

surface-to-surface_map The "*surface-to-surface map*" generator defines a data field on the domain bounded by two surfaces. The data values are interpolated using a user-defined function between the surfaces.

```
<MeshData>
  <mesh_data name="E" generator="surface-to-surface map" elem_set="Part1">
    <function type="math">x*x+1</function>
    <bottom_surface surface="surface1"/>
    <top_surface surface="surface2"/>
  <mesh_data>
</MeshData>
```

3.8.2 ElementData

This section defines data that will be mapped to the elements of a part. Currently, only predefined variables can be mapped (i.e. requires the *var* attribute). The element set that this data will be mapped to is defined via the *elem_set* attribute. The following table lists the currently supported predefined variables.

Property	Description	Data type/format
fiber	Specify a local fiber direction	vec3/const
shell thickness	Specify the shell element thickness	float/shape
MRVonMisesParameters	Von Mises Fibers coefficients kf and tp	vec2/const
mat_axis	Specify local element material axes	vec3/const

Some materials define spatially varying material parameters. Data to these types of parameters can be mapped using the *ElementData* section and the *var* attribute.

```
<MeshData>
  <ElementData var="shell thickness" elem_set="part1">
    <elem lid="1">1.0, 1.0, 1.0, 1.0</elem>
    <elem lid="2">1.0, 1.0, 1.0, 1.0</elem>
  </ElementData>
  <ElementData var="pre_stretch" elem_set="part2">
    <elem lid="1">1.05</elem>
    <elem lid="2">1.05</elem>
  </ElementData>
  <ElementData var="mat_axis" elem_set="part3">
    <elem lid="1">
      <a>1,0,0</a>
      <d>0,1,0</d>
    </elem>
    <elem lid="2">
      <a>1,1,0</a>
      <d>0,1,1</d>
    </elem>
  </ElementData>
</MeshData>
```

3.8.3 SurfaceData

This section allows users to define data that can be mapped to the surfaces of certain boundary conditions and loads. This section only defines user-defined data maps, i.e. the *name*, *data_type* and *data_format* attributes must be used. The surface is defined via the *surface* attribute.

```
<SurfaceData name="values" surface="surface1">
  <face lid="1">1.23</face>
  <face lid="2">3.45</face>
</SurfaceData>
```

The surface definition is defined in the *Mesh* section. Note that the ids refer to the local ids of the surface facets. By default, the *scalar* data type and *const* data format are assumed so only one value per facet is expected. Other data types and formats can be specified with the *data_type* and *data_format* attributes.

```
<SurfaceData name="data" data_type="vec3" surface="surface1">
  <face lid="1">0.0, 1.0, 0.0</face>
  <face lid="2">0.0, 2.0, 0.0</face>
</SurfaceData>
```

Optionally, the surface data may be described with a mathematical expression as a function of the initial coordinates (X,Y,Z) of the centroid of each face:

```
<SurfaceData name="inlet" data_type="scalar" generator="math" surface="surface1">
  <math>2*(1-X^2-Y^2)</math>
</SurfaceData>
```

3.8.4 EdgeData

This section allows users to define user-defined data maps that will be mapped to an edge defined in the Mesh section.

```
<EdgeData name="data" edge="edge1">
  <edge lid="1">1.0</edge>
  <edge lid="2">2.0</edge>
</EdgeData>
```

Notice that the *local* IDs are required here.

3.8.5 NodeData

This section allows users to define data that will be mapped to node sets.

```
<NodeData name="data" node_set="set1">
  <node lid="1">1.0</node>
  <node lid="2">2.0</node>
</NodeData>
```

For node data the *data_format* attribute, if specified, will be ignored. Optionally, the node data may be described with a mathematical expression as a function of the initial nodal coordinates (X,Y,Z):

```
<NodeData name="data" generator="math" node_set="set1">
  <math>1e-3*Y</math>
</NodeData>
```

3.9 Initial Section

The *Initial* section defines all initial conditions that may be applied to the analysis. An initial condition is defined via the *init* element and requires the *bc* attribute and *node_set* attribute. The *bc* attribute defines the degree of freedom to which the initial condition is applied. The *node_set* attribute defines the set of nodes that this initial condition affects. The value of the initial condition is then defined with the *value* element.

```
<init bc="vx" node_set="set1">
  <value>1.0</value>
</init>
```

3.9.1 The Prestrain Initial Condition

The prestrain initial condition can be used to accomplish one of two things. It can be used to convert a forward analysis in an equivalent prestrain analysis. Or it can be used to fix the prestrain gradient. In either case the current geometry is used as the new reference geometry of the following analysis step.

parameter	description	initial value
init	Initialize prestrain field	1 (=true)
reset	Make current geometry the reference geometry of the following steps	1 (=true)

The following example shows how a forward analysis can be converted to a prestrain analysis.

```
<ic type="prestrain">
  <init>1</init>
  <reset>1</reset>
</ic>
```

Note that this in itself may not be sufficient to define the equivalent prestrain analysis. For instance, if the forward model applied prescribed displacements, then these boundary conditions must be replaced with fixed boundary conditions.

If the *init* parameter is set to 0 (false), then the prestrain gradient will be fixated in the current geometry. This means that any remaining distortion will be applied to the prestrain correction factor before the current geometry is converted to the new reference geometry.

3.10 Boundary Section

The *Boundary* section defines all fixed and prescribed boundary conditions that may be applied to the geometry. Individual boundary conditions are defined via the *bc* tag and the particular boundary condition is defined via the *type* attribute. The following boundary condition types are currently supported.

fix Define a fixed boundary condition. A fixed boundary condition is usually identical to a zero prescribed boundary condition.

prescribe Define a prescribed boundary condition. The nodal values of a prescribed boundary condition are define by the user and can vary as a function of time and position.

rigid Define a rigid node set. The nodes in a rigid node set move with the rigid body to which they are assigned.

3.10.1 Prescribed Nodal Degrees of Freedom

Nodal degrees of freedom (dof) can be prescribed using the *prescribe* boundary condition. This element has two required attributes: the *type* is set to "prescribe" and the node set to which this boundary condition applies is defined vua *node_set*. The optional *name* attribute can be used to give the boundary condition a name. The value is defined via the *scale* parameter. (If omitted the default value is 1.0). The degree of freedom is defined via the *dof* parameter. A loadcurve can be associated with the scale parameter. The relative parameter defines wheter the values are absolute or relative to the current displacement.

```
<bc type="prescribe" node_set="nodeset1">
  <dof>x</dof>
  <scale lc="1">2.0</scale>
  <relative>0</relative>
</bc>
```

Here, *nodeset1* is the name of a node set defined in the Mesh section. See Section 3.6.3 for more information on how to define node sets. Node sets can also be defined via surfaces or element sets. To define a node set via a surface, use the following syntax.

```
node_set="@surface:surface1"
```

Here, *surface1* is a surface defined in the *Mesh* section. Similarly, defining a node set via an element set is done using *@elem_set:.*

The *dof* parameter specifies the particular degree of freedom. The following values are allowed:

x apply displacement in x-direction

y apply displacement in y-direction

z apply displacement in z-direction

sx apply shell back-face displacement in x-direction (new shell formulation)

sy apply shell back-face displacement in y-direction (new shell formulation)

sz apply shell back-face displacement in z-direction (new shell formulation)

u apply shell director component in x-direction (old shell formulation)

v apply shell director component in y-direction(old shell formulation)

w apply shell director component in z-direction(old shell formulation)

p apply prescribed effective fluid pressure (biphasic and multiphasic analyses)

T apply prescribed temperature (heat transfer analysis)

c apply prescribed effective solute concentration (solute analysis)

c[n] apply prescribed effective solute concentration on solute n (multiphasic analysis)

wx apply prescribed fluid velocity relative to mesh in x-direction (fluid and FSI analyses)

wy apply prescribed fluid velocity relative to mesh in y-direction (fluid and FSI analyses)

wz apply prescribed fluid velocity relative to mesh in z-direction (fluid and FSI analyses)

ef apply prescribed fluid dilatation (fluid analysis)

For solutes, replace "n" with the solute id from the global solute table (Section 3.4.2); for example, "c2".

The loadcurve for the scale parameter is specified with the *lc* attribute. The value of the *lc* attribute is the ID of the loadcurve that is defined in the *LoadData* section of the input file.

The optional *relative* parameter allows users to choose between absolute (default) and relative boundary conditions. Absolute boundary conditions assign the specified value to the desired nodal degree of freedom. Relative boundary conditions are meaningful only in multi-step analyses. When a nodal degree of freedom is specified to be relative at a particular step, the value prescribed for that node is superposed over the value of that degree of freedom at the end of the preceding step.

To define a different displacement value for each node, a *mesh_data* section needs to be defined.

```
<Boundary>
  <bc type="prescribe" node_set="set1">
    <dof>x</dof>
    <scale lc="1">2.0</scale>
    <relative>0</relative>
  </bc>
</Boundary>
<MeshData>
  <mesh_data param="fem.bc_prescribed[0]">
    <node lid="1">1.0</node>
    <node lid="2">2.0</node>
    <node lid="3">3.0</node>
  </mesh_data>
</MeshData>
```

Keep in mind that the *scale* parameter of the prescribed bc will scale the values defined in the mesh data section.

3.10.2 Fixed Nodal Degrees of Freedom

Degrees of freedom that are fixed (in other words, constrained, or are always zero) can be defined using the *fix* boundary condition:

```
<bc type="fix" set="nodeset">
  <dofs>x,y,z</dofs>
<bc>
```

The node set must be defined in the *Mesh* section.

The fix boundary condition can be assigned to multiple degrees of freedom of the node set and the list of degrees of freedom is defined via the *dofs* parameter.

Although the *prescribe* element with a value of zero for the *node* tags can also be used to fix a certain nodal degree of freedom, the user should use the *fix* element whenever possible, since this option causes the equation corresponding to the constrained degree of freedom to be removed from the linear system of equations. This results in fewer equations that need to be solved for and thus reduces the run time of the FE analysis.

3.10.3 Rigid Nodes

A node set can be attached to a rigid body using the *rigid* boundary condition. Rigid nodes are not assigned degrees of freedom.

```
<bc type="rigid" node_set="set1">
  <rb>2</rb>
</bc>
```

The *rb* parameter defines the material (which must be a “rigid body” material) that in turn defines the rigid body. The node set must be defined in the *Mesh* section.

3.11 Rigid Section

The *Rigid* section is used to define all rigid constraints, rigid body initial kinematics, and rigid connectors, and rigid joints.

3.11.1 Prescribed Rigid Body Degrees of Freedom

Rigid bodies are initially unconstrained which means they can move in all three directions and can rotate about all three axes. To constrain the degrees of freedom of a rigid body you can use the *rigid_body* element:

```
<rigid_body mat="<id>">
  <!-- constraints go here -->
</rigid_body>
```

The *mat* attribute defines the material (which must be rigid) that defines the rigid body.

The following table lists the elements that can be defined in the *rigid_body* element:

Tag	Description
fixed	Degree of freedom is fixed
prescribed	Degree of freedom is prescribed by user
force	A force is applied in direction of degree of freedom

All these tags require the *bc* attribute which defines the degree of freedom that will be constrained.

Bc	Description
x	Constrain the $x$degree of freedom
y	Constrain the $y$degree of freedom
z	Constrain the $z$degree of freedom
Rx	Prevent the rigid body from rotating around the $x-$axis
Ry	Prevent the rigid body from rotating around the $y-$axis
Rz	Prevent the rigid body from rotating around the $z-$axis

If the tag is *prescribed* or *force* then the *lc* attribute can be used to specify a load curve defining the amplitude of the displacement or force. The value is then interpreted as a scale factor. For all other types the value is ignored. The syntax and interpretation is the same for the other translation and rotation codes.

When the type is *force*, the force is applied at the center of mass for translational degrees of freedom and torque is applied around the center of mass for rotational degrees of freedom. The center of mass of a rigid body is either specified in the material definition or calculated automatically by FEBio.

Example:

```
<rigid_body mat="1">
  <prescribed bc="x" lc"1">2.0</prescribed>
  <fixed bc="y"/>
  <fixed bc="z"/>
```

```
  <fixed bc="Rx"/>
  <fixed bc="Ry"/>
  <fixed bc="Rz"/>
</rigid_body>
```

In this example the rigid body that corresponds to material definition *1* has a prescribed displacement defined for the $x$degree of freedom and has all other degrees of freedom fixed.

A force (torque) can be applied at the center of mass by setting the *type* attribute to *force*. Note that specifying a force (torque) will automatically free the corresponding translational (rotational) degree of freedom. For example, applying a force in the x-direction while keeping the y and $z$directions fixed and the rotational degrees of freedom free, can be done as follows:

```
<rigid_body mat="1" >
  <force bc="x" lc="1">1.0</force>
  <fixed bc="y"/>
  <fixed bc="z"/>
</rigid_body>
```

3.12 Loads Section

The *Loads* section defines all nodal, surface and body loads that can be applied to the model.

3.12.1 Nodal Loads

Nodal loads are applied by the *nodal_load* element. When the loads are applied to displacement degrees of freedom, the forces always point in the same direction and do not deform with the geometry (i.e. they are non-follower forces). For other degrees of freedom they define a constant normal flux.

```
<nodal_load bc="x" node_set="set1">
  <scale lc="1">1.0</scale>
  <value>3.14</value>
</nodal_load>
```

The *bc* attribute gives the degree of freedom. The following values are allowed:

x apply force in x-direction

y apply force in y-direction

z apply force in z-direction

p apply normal volumetric fluid flow rate

cn apply normal molar solute flow rate

t apply normal heat flux (heat transfer analysis)

For solutes, replace "n" with the solute id from the global solute table (Section 3.4.2); for example, "c2".

An optional *loadcurve* can be specified for the *scale* parameter with the *lc* attribute. If a loadcurve is not specified, the value will be automatically ramped from a value of 0 at time t =0 to the value specified in the xml file at the time corresponding to the end of the analysis.

The value of the *value* parameter (e.g. 3.14 in the example above) is the value for the nodal force. This value will be scaled by the *scale* parameter. Note that if a *loadcurve* is specified, this value scales the value determined by the *loadcurve*.

To define a different value for each node of the node set, define a *NodData* field in the *MeshData* section and reference it by defining the *node_data* attribute in the *value* parameter.

3.12.2 Surface Loads

A surface load can be applied using the *surface_load* element. This element takes two attributes, namely *type*, which defines the type of surface load that will be applied, and *surface* which defines the surface that this load will be applied to.

3.12.2.1 Pressure Load

Pressure loads are applied to the surface of the geometry and are defined by the *surface_load* element with the type attribute set to *pressure*. These pressure forces are also known as *follower forces*; they change direction as the body is deformed and, in this case, are always oriented along the local surface normal. The sign convention is so that a positive pressure will act opposite to the normal, so it will compress the material. The surface that the load is applied to is specified with the *surface* attribute.The surface must be defined in the *Mesh* section.

parameter	**Description**	default
pressure	The applied pressure values (1)	0 [**P**]
symmetric_stiffness	symmetric stiffness flag (2)	1
linear	linear flag (3)	0
shell_bottom	shell bottom flag (4)	0

Comments:

1. The *pressure* element defines the pressure value [**P**]. The optional parameter *lc* defines a loadcurve for the pressure evolution. If *lc* is not defined a constant pressure is applied.

2. The optional *symmetric_stiffness* parameter (0 or 1) determines whether to use the exact form of the stiffness matrix for this surface load (0=non-symmetric), or the symmetric form (1=default). The non-symmetric form is numerically more robust, but it may also require using a globally non-symmetric stiffness matrix (see Section 3.3.4).

3. If the optional *linear* parameter is set to 1, a constant, deformation independent pressure load is applied. This is not recommend for large deformations.

4. When the *shell_bottom* flag is set to 1, the surface is assumed to be a shell surface and the pressure is applied to the bottom part of the shell surface.

Example:

```
<surface_load type="pressure" surface="surface1">
  <pressure lc="1">1.0</pressure>
  <symmetric_stiffness>0</symmetric_stiffness>
</surface_load>
```

3.12.2.2 Traction Load

A traction load applies a traction to a surface. The direction of the traction remains unchanged as the mesh deforms.

```
<surface_load type="traction" surface="surface1">
  <scale lc="1">1.0</scale>
  <traction>0,0,1</traction>
</surface_load>
```

If a different needs to be specified for each facet, use the following syntax.

```
<surface_load type="traction" surface="surface1">
  <scale lc="1">1.0</scale>
  <traction surface_data="traction_value"/>
</surface_load>
```

The traction vector is determined by two quantities. The direction and magnitude is defined by the *traction* element. In addition, the magnitude can be scaled using the *scale* element. An optional load curve can be defined for the *scale* element using the *lc* attribute. This allows the traction load to become time dependent. If the *lc* attribute is omitted a constant traction load is applied.

3.12.2.3 Mixture Normal Traction

This section applies to biphasic, biphasic-solute, triphasic and multiphasic analyses. In a mixture of intrinsically incompressible solid and fluid constituents, the formulation adopted in FEBio implies that the total traction is a natural boundary condition (*FEBio Theory Manual*). If this boundary condition is not explicitly prescribed, the code automatically assumes that it is equal to zero. Therefore, boundaries of mixtures are traction-free by default.

The *mixture traction* $\mathbf{t}$ is the traction vector corresponding to the mixture (or total) stress $\boldsymbol{\sigma}$; thus $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$, where $\mathbf{n}$ is the outward unit normal to the boundary surface. Since $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}^e$, where p is the fluid pressure and $\boldsymbol{\sigma}^e$ is the *effective stress* resulting from strains in the solid matrix, it is also possible to represent the total traction as $\mathbf{t} = -p\mathbf{n} + \mathbf{t}^e$, where $\mathbf{t}^e = \boldsymbol{\sigma}^e \cdot \mathbf{n}$ is the *effective traction*. Currently, FEBio allows the user to specify only the normal component of the traction, either $t_n = \mathbf{t} \cdot \mathbf{n}$ (the normal component of the mixture traction) or $t_n^e = \mathbf{t}^e \cdot \mathbf{n}$ (the normal component of the effective traction):

A mixture normal traction is defined by the *surface_load* element using *normal_traction* for the type attribute.

```
<surface_load type="normal_traction" surface="surface1">
  <traction [lc="1"]>1.0</traction>
  <effective>1</effective>
  <linear>0</linear>
</surface_load>
```

The *traction* element defines the magnitude of the traction force. The optional attribute *lc* defines a loadcurve that controls the time dependency of the traction force magnitude. If omitted a constant traction is applied.

The *effective* element defines whether the traction is applied as an effective traction or a total mixture traction.

The *linear* element defines whether the traction remains normal to the deformed surface or the reference surface. If set to true the traction remains normal to the reference surface. When false it defines a follower force that remains normal to the deformed surface.

The *surface* element defines the surface to which the traction is applied. It consists of child elements defining the individual surface facets.

Unlike the mixture and effective traction, the fluid pressure p is a nodal variable (see Section 3.10.1). There may be common situations where the user must apply a combination of related fluid pressure and traction boundary conditions. For example, if a biphasic surface is subjected to a non-zero fluid pressure p_0, the corresponding boundary conditions are $p = p_0$ and $t_n = -p_0$ (or $t_n^e = 0$). In FEBio, both boundary conditions must be applied. For example:

```
<Boundary>
  <prescribed bc="p" node_set="set1">
    <scale lc="1">1.0</scale>
  </prescribed>
  <surface_load type="normal_traction" surface="surf1">
    <traction lc="1">-1.0</traction>
    <effective>0</effective>
    <linear>0</linear>
  </surface_load>
</Boundary>
<LoadData>
  <loadcurve id="1">
    <loadpoint>0,0</loadpoint>
    <loadpoint>1,2.0</loadpoint>
  </loadcurve>
</LoadData>
```

3.12.2.4 Fluid Flux

In a biphasic mixture of intrinsically incompressible solid and fluid constituents, the $\mathbf{u}-p$ formulation adopted in FEBio implies that the normal component of the relative fluid flux is a natural boundary condition. If this boundary condition is not explicitly prescribed, the code automatically assumes that it is equal to zero. Therefore, biphasic boundaries are impermeable by default. (To implement a free-draining boundary, the fluid pressure nodal degrees of freedom should be set to zero.)

The flux of fluid relative to the solid matrix is given by the vector $\mathbf{w}$. Since viscosity is not explicitly modeled in a biphasic material, the tangential component of $\mathbf{w}$ on a boundary surface may not be prescribed. Only the normal component of the relative fluid flux, $w_n = \mathbf{w}\cdot\mathbf{n}$, represents a natural boundary condition. To prescribe a value for w_n on a surface, use:

```
<surface_load type="fluidflux" surface="surf1">
  <flux [lc="1"]>1.0</flux>
  <linear>0</linear>
```

```
  <mixture>1</mixture>
</fluidflux>
```

The *flux* parameter defines the flux that will be applied to the surface. The optional parameter *lc* defines a loadcurve for the normal flux evolution. If omitted a constant fluid flux is applied.

When *linear* is set to zero (default) it means that the flux matches the prescribed value even if the surface on which it is applied changes in area as it deforms. Therefore, the net volumetric flow rate across the surface changes with changes in area. This type of boundary condition is useful if the fluid flux is known in the current configuration.

When *linear* is set to non-zero it means that the prescribed flux produces a volumetric flow rate based on the undeformed surface area in the reference configuration. Therefore, the flux in the current configuration does not match the prescribed value. This type of boundary condition is useful if the net volumetric flow rate across the surface is known. For example: Let Q be the known volumetric flow rate, let A_0 be the surface area in the reference configuration (a constant). Using *"linear"* means that the user prescribes Q/A_0 as the flux boundary condition. (However, regardless of the *type*, the fluid flux saved in the output file has a normal component equal to Q/A, where $A =$area in current configuration.)

Prescribing w_n on a free surface works only if the nodal displacements of the corresponding faces are also prescribed. If the nodal displacements are not known a priori, the proper boundary condition calls for prescribing the normal component of the mixture velocity, $v_n = (\mathbf{v}^s + \mathbf{w}) \cdot \mathbf{n}$. To prescribe the value of v_n on a surface, use

```
<surface_load type="fluidflux" surface="surf1">
  <flux lc="1">1.0</flux>
  <linear>0</linear>
  <mixture>1</mixture>
</surface_load>
```

For example, this boundary condition may be used when modeling a permeation problem through a biphasic material, when the upstream fluid velocity is prescribed, $v_n = v_0$. If the upstream face is free, the companion boundary condition would be to let $t_n^e = 0$ on that face as well.

3.12.2.5 Solute Flux

The molar flux of solute relative to the solid matrix is given by the vector $\mathbf{j}$. Since solute viscosity is not explicitly modeled in a biphasic-solute material, the tangential component of $\mathbf{j}$ on a boundary surface may not be prescribed. Only the normal component of the relative solute flux, $j_n = \mathbf{j} \cdot \mathbf{n}$, represents a natural boundary condition. To prescribe a value for j_n on a surface, use:

```
<surface_load type="soluteflux" surface="surface1">
  <flux [lc="1"]>1.0</flux>
  <linear>0</linear>
  <solute_id>1</solute_id>
</ surface_load>
```

The optional parameter *solute_id* specifies to which solute this flux condition applies, referencing the corresponding list in the Globals section (Section 3.4.2). If *solute_id* is not defined, the default value is 1.

The *flux* element defines the flux magnitude. The optional parameter *lc* defines a loadcurve for the normal flux evolution. If omitted a constant flux is applied.

When *linear* is set to 0 (default) it means that the flux matches the prescribed value even if the surface on which it is applied changes in area as it deforms. Therefore, the net molar flow rate across the surface changes with changes in area. This type of boundary condition is useful if the solute molar flux is known in the current configuration.

When *linear* is set to non-zero it means that the prescribed flux produces a molar flow rate based on the undeformed surface area in the reference configuration. Therefore, the flux in the current configuration does not match the prescribed value. This type of boundary condition is useful if the net molar flow rate across the surface is known. For example: Let Q be the known molar flow rate (in units of moles per time [**n**/**t**]), let A_0 be the surface area in the reference configuration (a constant). Using *"linear"* means that the user prescribes Q/A_0 as the flux boundary condition (in units of moles per area per time [**n**/**L**^{2}·**t**]). However, regardless of the *type*, the solute molar flux saved in the output file has a normal component equal to Q/A, where A =area in current configuration.

3.12.2.6 Heat Flux

A heat flux can be defined for heat transfer analyses using the *surface_load* element with type set to *heatflux* element.

```
<surface_load type="heatflux" surface="surface1">
  <flux [lc="1"]>1.0</flux>
</surface_load>
```

The heat flux element takes two parameters, namely *flux* which defines the flux that will be applied. It has an optional *lc* attribute which defines the load curve for this parameter. If omitted, a constant heat flux will be applied. The other (optional) parameter is the *value* parameter which can be used to define a different flux value for each surface facet.

3.12.2.7 Convective Heat Flux

A convective heat flux can be defined to a surface that is cooled (or heated) by exposure to an ambient temperature.

```
<surface_load type="convective_heatflux" surface="surf1">
  <Ta [lc="1"]>1.0</Ta>
  <hc>1.0</hc>
</surface_load>
```

The *hc* parameter defines the heat transfer coefficient. The ambient temperature is defined by the *Ta* parameter. It takes an optional load curve defined through the *lc* attribute. The *value* parameter with the *surface_data* attribute can be defined to define a different temperature value for each surface facet (Section 3.8.1).

3.12.2.8 Fluid Traction

In a fluid or fluid-FSI analysis, the Cauchy stress is given by $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}$, where p is the elastic pressure and $\boldsymbol{\tau}$ is the viscous stress. The traction on a fluid surface with outward normal $\mathbf{n}$ is given

by $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n} = -p\mathbf{n} + \mathbf{t}^\tau$, where $\mathbf{t}^\tau = \boldsymbol{\tau} \cdot \mathbf{n}$ is the viscous component of the traction. The *fluid traction* surface load prescribes $\mathbf{t}^\tau$ on a boundary surface.

```
<surface_load type="fluid traction" surface="surface1">
  <scale lc="1">1.0</scale>
  <traction>0,0,1</traction>
</surface_load>
```

If a different vector value needs to be specified for each facet, use the following syntax,

```
<surface_load type="fluid traction" surface="surface1">
  <scale lc="1">1.0</scale>
  <traction surface_data="traction_value"/>
</surface_load>
```

and provide the facet values in a user-defined *SurfaceData* map (Section 3.8.1).

3.12.2.9 Fluid Normal Traction

In a fluid or fluid-FSI analysis, the normal component $t_n^\tau = \mathbf{t}^\tau \cdot \mathbf{n}$ of the viscous traction $\mathbf{t}^\tau$ (Section 3.12.2.8) may be prescribed on a boundary surface in a fluid analysis. The *fluid normal traction* surface load prescribes t_n^τ on a boundary surface.

```
<surface_load type="fluid normal traction" surface="surface1">
  <scale [lc="1"]>1.0</scale>
  <traction>1</traction>
</surface_load>
```

If a different scalar value needs to be specified for each facet, use the following syntax,

```
<surface_load type="fluid normal traction" surface="surface1">
  <scale [lc="1"]>1.0</scale>
  <traction surface_data="traction_value"/>
</surface_load>
```

and provide the facet values in a user-defined *SurfaceData* map (Section 3.8.1).

3.12.2.10 Fluid Backflow Stabilization

In a fluid or fluid-FSI analysis, this boundary condition prescribes the normal component of the viscous traction (Section 3.12.2.8), $t_n^\tau = \mathbf{t}^\tau \cdot \mathbf{n}$, such that it opposes backflow, i.e., when $v_n = \mathbf{v} \cdot \mathbf{n}$ is negative. Specifically, $t_n^\tau = \beta \rho_r v_n^2$ when $v_n < 0$ and 0 otherwise, where β is a unitless user-defined parameter (typical values may range from 0 to 1) and ρ_r is the referential fluid density.

```
<surface_load type="fluid backflow stabilization" surface="surface1">>
<beta [lc="1"]>1</beta>
</surface_load>
```

3.12.2.11 Fluid Tangential Stabilization

In a fluid or fluid-FSI analysis, this boundary condition prescribes the tangential component of the viscous traction (Section 3.12.2.8), $\mathbf{t}_t^\tau = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \mathbf{t}^\tau$, such that it opposes the tangential fluid flow $\mathbf{v}_t = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \mathbf{v}$ on the selected boundary surface, with $\mathbf{n}$ representing the outward normal to this surface. Specifically, $\mathbf{t}_t^\tau = -\beta \rho_r \left|\mathbf{v}_t\right| \mathbf{v}_t$, where β is a unitless user-defined parameter (typical values may range from 0 to 1) and ρ_r is the referential fluid density.

```
<surface_load type="fluid tangential stabilization" surface="surface1">
<beta [lc="1"]>1</beta>
</surface_load>
```

3.12.2.12 Fluid Normal Velocity

In a fluid or fluid-FSI analysis the fluid velocity relative to the mesh, $\mathbf{w}$, on a boundary surface with outward normal $\mathbf{n}$ may be decomposed into the normal component, $w_n = \mathbf{w} \cdot \mathbf{n}$, and tangential component, $\mathbf{w}_\tau = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \mathbf{w} = \mathbf{w} - w_n \mathbf{n}$. The surface load *fluid normal velocity* may be used to prescribe a desired value of w_n on a boundary surface.

```
<surface_load type="fluid normal velocity" surface="surface1">
  <value [lc="1"]>1.0</value>
  <velocity>1</velocity>
</surface_load>
```

Optionally, FEBio can generate a parabolic velocity profile over the named surface, This option can be turned on using the *parabolic* element (0=default, 1=parabolic). In this case, the *velocity* element provides the average value of this parabolic velocity profile, while *value* remains a scale factor optionally tied to a loadcurve. The parabolic profile is calculated under the assumption of steady Poiseuille flow in an infinite tube whose cross-section has the shape of the named surface. All nodes located along the curve boundary of this surface are prescribed zero normal velocity.

```
<surface_load type="fluid normal velocity" surface="surface1">
  <velocity lc=”1”>-1.0</velocity>
  <parabolic>1</parabolic>
</surface_load>
```

If an arbitrary distribution with different scalar value needs to be specified for each facet, use the following syntax,

```
<surface_load type="fluid normal velocity" surface="surface1">
  <value surface_data="inlet"/>
  <velocity lc="1">-1.0</value>
</surface_load>
```

and provide the facet values in a user-defined *SurfaceData* map with *name="inlet"* and *data_type="scalar"* (Section 3.8.1).

By default, this condition only prescribes the natural boundary condition w_n, leaving $\mathbf{w}_\tau$ free. Optionally, it is possible to also enforce $\mathbf{w}_\tau = \mathbf{0}$ by prescribing essential boundary conditions on the wx, wy and wz components of $\mathbf{w} = w_n \mathbf{n}$ at the nodes of each facet, based on the value of $\mathbf{n}$ at each node (obtained by averaging $\mathbf{n}$ from adjoining facets). This option may be turned on using the *prescribe_nodal_velocities* element (0=default, 1=prescribed), for example,

```
<surface_load type="fluid normal velocity" surface="surface1">
  <velocity>-1.0</velocity>
  <prescribe_nodal_velocities>1</prescribe_nodal_velocities>
</surface_load>
```

3.12.2.13 Fluid Velocity

In a fluid or fluid-FSI analysis, this boundary condition prescribes the fluid velocity vector relative to the mesh, $\mathbf{w}$, on a named surface, simultaneously satisfying the natural boundary condition for $w_n = \mathbf{w} \cdot \mathbf{n}$ and prescribing essential boundary conditions on the wx, wy and wz components of $\mathbf{w}$ at the nodes of each facet, based on the value of $\mathbf{n}$ at each node (obtained by averaging $\mathbf{n}$ from adjoining facets).

```
<surface_load type="fluid velocity" surface="surface1">
  <scale lc="1">1.0</scale>
  <velocity>0,0,1</velocity>
</surface_load>
```

If a different vector value needs to be specified for each facet, use the following syntax,

```
<surface_load type="fluid velocity" surface="surface1">
  <scale lc="1">1.0</scale>
  <velocity surface_data="inlet"/>
</surface_load>
```

and provide the facet values in a user-defined *SurfaceData* map with *name="inlet"* and *data_type="vec3"* (Section 3.8.1).

3.12.2.14 Fluid Rotational Velocity

This boundary condition prescribes a rotational velocity on an axisymmetric surface. It is the user's responsibility to ensure that the surface is axisymmetric. The angular velocity $\boldsymbol{\omega} = \omega\mathbf{n}$ is prescribed by specifying the angular speed ω and the unit vector along the axis of rotation (axis of symmetry) $\mathbf{n}$. The user-defined vector $\mathbf{n}$ is automatically normalized. If the axis does not pass through the origin, the user may specify any point $\mathbf{p}$ on the axis. The fluid velocity relative to the mesh, $\mathbf{w}$, for nodes on the selected surface is evaluated from $\mathbf{w} = \boldsymbol{\omega} \times \mathbf{r}$, where $\mathbf{r} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot (\mathbf{x} - \mathbf{p})$ is the shortest vector from the axis to the node and $\mathbf{x}$ is the nodal position.

```
<surface_load type="fluid rotational velocity" surface="FluidRotationalVelocity01">
<angular_speed lc="1">1</angular_speed>
<axis>0,0,1</axis>
<origin>0,0,0</origin>
</surface_load>
```

Though this boundary condition may be used in fluid-FSI analyses, it is most relevant for standard fluid analyses where the mesh is stationary.

3.12.2.15 Fluid Resistance

In a fluid or fluid-FSI analysis, this boundary condition prescribes an elastic pressure $p = RQ + p_0$ on a surface, where R is the flow resistance and Q is the volumetric flow rate across the surface (calculated internally); p_0 is an optional offset pressure. The pressure p is converted to a dilatation and prescribed as an essential boundary condition at the nodes of the facets.

```
<surface_load type="fluid resistance" surface="surface1">
  <R lc="1">7.93e+07</R>
  <pressure_offset lc="2">10640</pressure_offset>
<surface_load>
```

3.12.2.16 Fluid-FSI Traction

In a fluid-FSI analysis, the fluid traction across an interface with a solid domain must be prescribed explicitly as a traction boundary condition on the solid domain. Otherwise, the solid domain cannot sense the fluid pressure and viscous traction. Users must identify each surface on which this FSI surface load must be prescribed. There are no user-defined parameters for this surface load.

```
<surface_load type="fluid-FSI traction" surface="surface1">
<surface_load>
```

This surface load must also be prescribed on free fluid surfaces (such as the surface of the fluid in open channel flow) to allow those surfaces to deform in response to the fluid stresses (e.g., producing surface waves). (Do not apply this surface load on inlet or outlet boundaries through which fluid flows.)

3.12.3 Body Loads

A body load can be used to define a source term to the model. The following sections define the different type of body loads that can be applied. In the case of body forces, these body loads represent the body force per mass, $\mathbf{b}$, which appears in the momentum balance as

$$\rho\mathbf{a} = \operatorname{div}\boldsymbol{\sigma} + \rho\mathbf{b}\,,$$

where ρ is the mass density, $\mathbf{a}$ is the acceleration (set to zero in quasi-static analyses), and $\boldsymbol{\sigma}$ is the Cauchy stress tensor.

3.12.3.1 Constant Body Force

This constant body force per mass $\mathbf{b}$ is defined as a 3D vector. Each component can be associated with a load curve to define a time dependent body force. Only the non-zero components need to be defined. This type of body force is spatially homogeneous, though it may vary with time when associated with a load curve:

```
<body_load type="const">
  <x lc="1">1.0</x>
  <y lc="2">1.0</y>
  <z lc="3">1.0</z>
</body_load>
```

The *lc* attribute defines the load curve to use for the corresponding component. The values of the components can be used to define scale factors for the load values.

3.12.3.2 Non-Constant Body Force

This body force per mass $\mathbf{b}$ may be spatially inhomogeneous. The spatial inhomogeneity may be specified using a formula with variables x, y, z. For example:

```
<body_load type="non-const">
  <x>x+y+z</x>
  <y>x-y-z</y>
  <z>x*x+z</z>
</body_load>
```

3.12.3.3 Centrifugal Body Force

A centrifugal body force per mass $\mathbf{b} = \omega^2 r \mathbf{e}_r$ may be used for bodies undergoing steady-state rotation with angular speed ω about a rotation axis directed along $\mathbf{n}$ and passing through the rotation center $\mathbf{c}$. Here, r represents the distance of each material point from the axis of rotation, and $\mathbf{e}_r$ is the radial unit vector from the axis of rotation, both of which are calculated internally from the knowledge of $\mathbf{n}$ and $\mathbf{c}$.

```
<body_load type="centrifugal">
  <angular_speed>1.0</angular_speed>
  <rotation_axis>0.707,0.707,0</rotation_axis>
  <rotation_center>0,0,0</rotation_center>
</body_load>
```

3.12.3.4 Heat Source

A heat source can be defined using the *heat_source* type.

```
<body_load type="heat_source">
  <Q>1.0</Q>
</body_load>
```

3.12.3.5 Surface Attraction

A surface attraction body force can be used to attract a mesh toward a boundary surface, for the purpose of creating a mesh bias. This can be useful for fluid analyses where a finer mesh is needed in the vicinity of a no-slip boundary. The benefit of this tool over other existing tools for creating a biased mesh is its ability to work with structured and unstructured meshes, as well as linear and higher-order elements.

For each element in the mesh, its shortest distance r to the selected boundary surface is evaluated using a surface projection algorithm. Then, an attractive body force per mass,

$$\mathbf{b} = s \exp\left(-\frac{r}{\rho}\right) \mathbf{n}$$

is evaluated along the unit vector $\mathbf{n}$ directed along the shortest projection distance. Here, ρ is a characteristic boundary layer thickness (*blt*) and s is a scale factor for the body force (*bsf*), whose value may be adjusted relative to account for the stiffness of the elastic solid material assigned to the mesh.

```
<body_load type="surface attraction" elem_set="EB1" surface="PressureLoad1">
    <blt>0.5</blt>
    <bsf lc="1">20</bsf>
    <search_radius>0.1</search_radius>
    <search_tol>0.01</search_tol>
</body_load>
```

Note that this body force requires the specification of an attractive surface; optionally, it also accepts the specification of the element set subjected to this attractive body force. The *search_radius* and *search_tol* parameters are used for the projection algorithm. They have the same meaning as in Section 3.13.1.

3.13 Contact Section

The *Contact* section defines all the contact interfaces. Contact boundary conditions are defined with the *contact* sub-element. The *type* attribute specifies the type of contact interface that is defined. The *surface_pair* attribute defines the surface pair to use for this contact definition. The surface pair is defined the the *Mesh* section. For example:

```
<contact type="sliding_with_gaps" surface_pair="contact1">
  <!-- parameter go here -->
</contact>
```

The *type* can be one of the following options:

Type	Description
sliding-node-on-facet, sliding-facet-on-facet, sliding-elastic, sliding-biphasic, sliding-biphasic-solute, sliding-multiphasic	A sliding interface that may separate (with biphasic contact for *sliding*-biphasic, biphasic-solute contact for *sliding-biphasic-s*olute, and multiphasic contact for *sliding-multiphasic*)
rigid_wall	A sliding interface with rigid wall as secondary surface
rigid_joint	A joint between two rigid bodies
tied,sticky, tied-biphasic	A tied interface (solid-solid, solid-rigid, solid-biphasic, rigid-biphasic) or tied-biphasic interface (biphasic-biphasic).

3.13.1 Sliding Interfaces

A sliding interface can be used to setup a non-penetration constraint between two surfaces. As of version 1.2, three different sliding contact algorithms are available. Although all three are based on the same contact enforcement method, they all differ slightly in their implementation and have been shown to give different performance for different contact scenarios. Each sliding contact implementation is identified by a different *type* attribute.

sliding-node-on-facet (N2F) This is FEBio's original implementation of sliding contact. It is based on Laursen's contact formulation [39] which poses the contact problem as a nonlinear constrained optimization problem. In FEBio, the Lagrange multipliers that enforce the contact constraints are computed either using a penalty method or the augmented Lagrangian method.

sliding-facet-on-facet (F2F) This implementation is identical to the *sliding_with_gaps* implementation but uses a more accurate integration rule: where the former method uses nodal integration, this method uses Gaussian quadrature to integrate the contact equations. This method has been demonstrated to give additional stability and often converges when the former method does not.

sliding-elastic (SE) This sliding contact interface also uses facet-on-facet contact but differs in the linearization of the contact forces, which results in a different contact stiffness matrix

compared to the previous two methods. It can be used for frictionless or frictional contact. It may optionally be set to sustain tension to prevent contact surfaces from separating along the direction normal to the interface, while still allowing tangential sliding. This method sometimes performs better than the previous two methods for problems that are dominated by compression. However, the formulation is inherently non-symmetric and therefore will require additional memory and running time. A symmetrized version of this implementation is available (see below), but the symmetric version does not converge as well as the non-symmetric version.

sliding-biphasic (SBP) This method extends the *sliding-elastic* algorithm to support frictionless biphasic contact (see the next section). This method is described in detail in [9].

sliding-biphasic-solute (SBS) This method is similar to *sliding-biphasic*. This contact implementation supports biphasic-solute contact (see the next section) [12]. When using biphasic-solute materials, the non-symmetric version must be used.

sliding-multiphasic (SMP) This method is similar to *sliding-biphasic-solute*. This contact implementation supports multiphasic contact (see the next section) [12]. When using multiphasic materials, the non-symmetric version must be used.

The following table lists the properties that are defined for sliding interfaces. It is important to note that the three different sliding implementations cannot be used interchangeably: not all features are available for each method. The third, fourth and fifth column indicate if a parameter is available for a particular implementation.

Parameter	**Description**	**N2F**	**F2F**	**SE**	**SBP SBS SMP**	**Default**
penalty	normal penalty scale factor (1)	•	•	•	•	1.0
auto_penalty	auto-penalty calculation flag (2)	•	•	•	•	0
update_penalty	updated auto-penalty calculation at each step (2)		•	•	•	0
two_pass	two-pass flag (3)	•	•	•	•	0
laugon	augmented Lagrangian flag (4)	•	•	•	•	0
tolerance	aug. Lagrangian convergence tolerance (4)	•	•	•	•	1.0
gaptol	tolerance for gap value (4)	•	•	•	•	0.0 (off)
minaug	minimum number of augmentations (4)	•	•	•		0
maxaug	maximum number of augmentations (4)	•	•	•		10
fric_coeff	frictional coefficient (5)	•		•		0.0
fric_penalty	tangential penalty factor (5)	•				0.0
ktmult	tangential stiffness multiplier (5)	•		•		1.0

seg_up	maximum number of segment updates (6)	•		•		0 (off)
smooth_aug	smoothed Lagrangian augmentation (7)		•	•	•	0 (off)
symmetric_stiffness	symmetric stiffness matrix flag (8)			•	•	0
search_tol	Projection search tolerance (9)	•	•	•	•	0.01
search_radius	search radius (10)		•	•	•	1.0
tension	tension flag (11)			•		0

Comments:

1. If the augmented Lagrangian flag is turned off (see comment 4), the penalty method is used to enforce the contact constraint. In this method, the contact traction is determined by the gap (i.e. penetration distance) multiplied by the user-defined *penalty* factor. In the augmented Lagrangian method, the *penalty* parameter is also used but has a slightly different meaning. In this case, it scales the Lagrange multiplier increment. Due to the different meanings, the user might have to adjust the penalty factor when switching between penalty method and augmented Lagrangian method. In general the penalty method requires a larger penalty factor to reach the same gap than the augmented Lagrangian method. See comment 4 for more information on when to use which method.

2. Choosing a good initial penalty parameter can often be a difficult task, since this parameter depends on material properties as well as on mesh dimensions. For this reason, an algorithm has been implemented in FEBio that attempts to calculate a good initial value for the penalty factor $\varepsilon_i$for a particular node/integration piont i on the contact interface:

$$\varepsilon_i = \frac{EA}{V}.$$

   Here, A is the area of the element the integration point belongs to, V is the element volume and E is a measure of the elasticity modulus, which is calculated from the elasticity tensor of the element. Although the meaning of E depends on the precise material formulation, in general one can regard it as a measure of the small strain Young's modulus of the material, when *update_penalty* is 0. If update_penalty is set to 1, E is recalculated at each iteration to account for the current deformation.

   To use this feature, add the following element to the contact section:

```
<auto_penalty>1</auto_penalty>
```

   When the auto-penalty flag is on, the value of the *penalty* parameter serves as a scale factor for the automatically-calculated penalty factor.

3. Each sliding interface consists of a *primary* surface and a *secondary* surface. The primary surface is the surface over which the contact equations are integrated and on which the contact tractions are calculated. The secondar surface is used to measure the gap function

and to define the necessary kinematic quantities such as surface normals and tangents. This approach is usually referred to as the *single-pass* method. When using the single-pass algorithm, the results can be influenced by the choice of primary and secondary surfaces. It is best to use the most tessellated surface as the primary and the coarsest as the secondary surface. To resolve the bias issue, one can also use a *two-pass* algorithm for enforcement of the contact constraint. In this case, a single pass is performed first, after which the primary and secondary surfaces are swapped and another pass is performed. When using the two-pass method, the definition of primary and secondary surfaces is arbitrary. In most problems, the single pass is sufficient to enforce contact; with a judicious choice of primary-secondary pair and contact parameters, good results can be obtained. If however, the single pass does not give good answers, for example, when due to the geometry's curvature the gap cannot be small enough with a single pass, the two-pass method can be used, although at the expense of more calculations.

If one of the contacting surfaces is rigid, a slightly different approach is recommended. In this case, it is best to pick the rigid surface as the secondary surface and to use a single pass algorithm. The reason is that the nodal degrees of freedom on the rigid surface are condensed to the rigid degrees of freedom and if the rigid surface is the primary surface, the reaction forces may not propagate correctly to the secondary surface. This is especially true if the rigid degrees of freedom are fixed.

4. In the presence of a sliding interface (and other contact interfaces), FEBio needs to calculate the contact tractions that prevent the two participating surfaces from penetrating. In general these tractions can be found using the method of Lagrange multipliers. However, the direct calculation of these multipliers has several computational disadvantages and therefore FEBio approximates the multipliers using one of two alternative methods: the penalty method and the augmented Lagrangian method. In the former method, the multipliers are approximated by the gap (i.e. penetration distance) scaled by a suitably chosen penalty factor. In many cases, this method is sufficient to get good results. Since the correctness of a contact solution is directly determined by the amount of penetration at the converged state, the user has direct control over the quality of the solution. By increasing the penalty factor, the penetration is reduced. However, in some cases, especially in large compression problems, the penalty factor required to achieve an acceptable amount of penetration has to be so large that it causes numerical instabilities in the non-linear solution algorithm due to ill-conditioning of the stiffness matrix. In these cases, the augmented Lagrangian method might be a better choice. In this method, the multipliers are determined iteratively where, in each iteration, the multiplier's increments are determined with a penalty-like method. The advantage of this method is twofold: due to the iterative nature, the method will work with a smaller penalty factor, and in the limit, the exact Lagrange multipliers can be recovered.

   To turn on the augmented Lagrangian method, simply add the following line to the contact section:

   ```
   <laugon>1</laugon>
   ```

   To turn off the augmented Lagrangian method, either set the value to 0 or remove the parameter altogether. The convergence tolerance is set as follows:

   ```
   <tolerance>0.01</tolerance>
   ```

With this parameter set, the augmented Lagrangian method will iterate until the relative increment in the multipliers is less than the tolerance. For instance, setting the tolerance parameter to 0.01 implies that the augmented Lagrangian method will converge when there is less than a 1% change in the L2 norm of the augmented Lagrangian multiplier vector between successive augmentations. Alternatively, the user can also specify a tolerance for the gap value. In this case, the iterations will terminate when the gap norm, which is defined as the averaged L2 norm, ($\sqrt{\sum_i < g_i >^2}/N$, $< \cdot >$the Macauley Bracket) is less than the user-specified value:

```
<gaptol>0.001</gaptol>
```

However, one must be careful when specifying a gap tolerance. First note that the gap tolerance is an absolute value (unlike the *tolerance* which is a relative value), so this parameter depends on the dimensions of the model. Also, there are cases when a gap tolerance simply cannot be reached due to the geometry of the model in which case the augmentations may never converge.

Note that both convergence parameters may be defined at once. In that case, FEBio will try to satisfy both convergence criteria. On the other hand, setting a value of zero will turn off the convergence criteria. For example, the default value for *gaptol* is zero, so that FEBio will not check the gap norm by default.

Finally, the *minaug* and *maxaug* can be used to set a minimum and maximum number of augmentations. When the *maxuag* value is reached, FEBio will move on to the next timestep, regardless of whether the force and gap tolerances have been met. When specifying a value for *minaug*, FEBio will perform at least minaug augmentations.

5. The *sliding-node-on-facet* and *sliding-elastic* contact implementations are currently the only contact algorithms that supports friction. For *node-on-facet*, three parameters control the frictional response: *fric_coeff* is the material's friction coefficient and its value must be in the range from 0.0 to 1.0; *fric_penalty* is the penalty factor that regulates the tangential traction forces, much like the *penalty* parameter regulates the normal traction force component; the parameter *ktmult* is a scale factor for the tangential stiffness matrix. It is default to 1.0, but it is observed that reducing this value might sometimes improve convergence. For *sliding-elastic*, only *fric_coeff* is needed to use frictional contact. Frictional contact is inherently dissipative and thus history-dependent. The solution may vary with the size of time increments, the cycle of loading, or Lagrangian augmentations (when *laugon*=1).

6. In a contact problem, FEBio calculates the projection of each node of the primary surface onto the secondary surface. As a node slides across the secondary surface, the corresponding surface facet can change. However, in some cases, switching facets is undesirable since it might cause instabilities in the solution process or a state in which the node oscillates continuously between two adjacent facets and thus prevents FEBio from meeting the displacement convergence tolerance. The parameter *seg_up* allows the user to control the number of segment updates FEBio will perform during each time step. For example, a value of 4 tells FEBio it can do the segment updates during the first four iterations. After that, nodes will not be allowed to switch to new segments. The default value is 0, which means that FEBio will do a segment update each iteration of each timestep.

7. The augmented Lagrangian method may produce a non-smooth contact pressure distribution at the contact surface, even though stresses within the underlying elements may

remain relatively smoother. Turning this flag on changes the method of updating the Lagrange multiplier to use the projection of the element stress to the corresponding contact face. This feature only works with some element types (HEX8G8, HEX8G1, TET4G4, TET4G1, PENTA6G6, TET10G1, TET10G4, TET10G8, TET10GL11, TET15G4, TET15G8, TET15G11, TET15G15, PYRA5G8).

8. The *sliding-elastic, sliding-biphasic*, *sliding-biphasic-solute* and *sliding-multiphasic* contact implementations for sliding contact are inherently non-symmetric formulations. Symmetrized versions of these algorithms do not perform as well as the nonsymmetric version so it is recommended to use the latter. The following line in the *contact* element controls which version of the algorithm is used.

```
<symmetric_stiffness>0</symmetric_stiffness>
```

A value of 1 uses the symmetric version, whereas a value of 0 uses the non-symmetric version. A similar line may be included in the *Control* element to use a non-symmetric global stiffness matrix. In some cases, a non-symmetric contact stiffness may converge well even when the global stiffness matrix is symmetric.

9. The *search_tol* parameter defines the search tolerance of the algorithm that projects nodes of the primary surface onto facets of the secondary syrface. A node that falls outside an element, but whose distance to the closest element's edge is less than the search tolerance is still considered inside. This can alleviate convergence problems when nodes are projected onto edges of elements and due to numerical error may be projected outside the surface.

10. The *search_radius* is a scale factor which multiplies the diagonal length of the model's bounding box to produce a dimensional search radius used by the algorithm that projects points onto facets. When the distance between the point and the facet exceeds the dimensional search radius, that projection is ignored. This can alleviate convergence problems when surfaces have multiple folds and the projection produces multiple solutions, only one of which (the closest distance) is valid.

11. The *tension* flag determines whether the contact interface can sustain tension and compression (*tension*=1) or only compression (*tension*=0).

3.13.2 Biphasic Contact

The *sliding-biphasic* implementation for sliding interfaces can deal with biphasic contact surfaces (including biphasic-on-biphasic, biphasic-on-elastic, biphasic-on-rigid) [9]. It allows for the possibility to track fluid flow across the contact interface. In other words, fluid can flow from one side of the contact interface to the other when both contact surfaces are biphasic. To use this feature, the user must define an additional contact parameter, namely:

```
<pressure_penalty>1.0</pressure_penalty>
```

In the same way that the *penalty* parameter controls the contact tractions, this parameter controls the penalty value that is used to calculate the Lagrange multipliers for the pressure constraint. If the *laugon* flag is set, the augmented Lagrangian method is used to enforce the pressure constraint.

And if the *auto_penalty* flag is defined (which is the recommended approach), an initial guess for the pressure penalty is calculated automatically using the following formula:

$$\varepsilon_p = \frac{kA}{V},$$

where A is the element's area, V is the element's volume and k is a measure of the permeability which is defined as one third of the trace of the material's initial permeability tensor.

When either contact surface is biphasic, the surface outside the contact area(s) is automatically set to free-draining conditions (equivalent to setting the fluid pressure to zero).

When performing biphasic-solute-on-rigid contact, a two-pass analysis should not be used; the biphasic-solute surface should be the primary surface.

3.13.3 Biphasic-Solute and Multiphasic Contact

The *sliding-biphasic-solute* implementation for sliding interfaces can deal with biphasic-solute contact surfaces (including biphasic-solute-on-biphasic-solute, biphasic-solute-on-biphasic, biphasic-solute-on-elastic, biphasic-solute-on-rigid) and the *sliding-multiphasic* contact interface can similarly deal with multiphasic contact surfaces. These contact interfaces allow for the possibility to track fluid and solute flow across the contact interface [12]. In other words, fluid and solute can flow from one side of the contact interface to the other. To use this feature, the user must define additional contact parameters, namely:

```
<pressure_penalty>1.0</pressure_penalty>
<concentration_penalty>1.0</concentration_penalty>
<ambient_pressure>0</ambient_pressure>
<ambient_concentration>0</ambient_concentration> (for sliding-biphasic-solute)
```

or

```
<ambient_concentration sol="id">0</ambient_concentration> (for sliding-multiphasic)
```

In the same way that the *penalty* parameter controls the contact tractions, these penalty parameters control the penalty values that are used to calculate the Lagrange multipliers for the pressure and concentration constraints. If the *laugon* flag is set, the augmented Lagrangian method is used to enforce the pressure and concentration constraints. And if the *auto_penalty* flag is defined, an initial guess for the pressure and concentration penalty is calculated automatically using the following formulas:

$$\varepsilon_p = \frac{k \cdot A}{V}, \quad \varepsilon_c = \frac{d \cdot A}{V},$$

where A is the element's area, V is the element's volume, k is a measure of the fluid permeability which is defined as one third of the trace of the material's initial permeability tensor, and d is a measure of the solute diffusivity which is defined as one third of the trace of the material's initial diffusivity tensor.

When either contact surface is biphasic-solute or multiphasic, the surface outside the contact area(s) is automatically set to ambient conditions (equivalent to setting the effective fluid pressure and effective solute concentration to the <ambient_pressure> and <ambient_concentration> values, respectively). Ambient conditions may also be associated with a load curve, for example:

```
<ambient_pressure lc="2">1.0</ambient_pressure>
<ambient_concentration lc="3">1.0</ambient_concentration>
```

When performing biphasic-solute-on-rigid or multiphasic-on-rigid contact, a two-pass analysis should not be used; the rigid surface should be the secondary surface.

3.13.4 Rigid Wall Interfaces

A rigid wall interface is similar to a sliding interface, except that the secondary surface is a rigid wall. The following properties are defined for rigid wall interfaces:

Parameter	Description	Default
laugon	Augmented Lagrangian flag	0 (false)
tolerance	augmentation tolerance	0.01
penalty	penalty factor	1.0
plane	the plane equation for the rigid wall	N/A
offset	the normal offset of the plane defined by the *plane* parameter	0.0

The *plane* property defines the reference plane for the rigid wall. Its value is an array of four values:a, b, c, d_0. The actual plane is defined by specifying the *offset* to the reference plane. The offset parameter takes a loadcurve as an optional attribute to define the motion of the plane as a function of time. The loadcurve defines the offset h from the initial position in the direction of the plane normal:

$$ax + by + cz + d\,(t) = 0, \quad d\,(t) = d_0 + h\,(t)$$

So, for example, a rigid wall that initially lies in the xy-coordinate plane and moves in the z-direction would be specified as follows:

```
<plane>0,0,1,0</plane>
<offset lc="1">1.0</offset>
```

3.13.5 Tied Interfaces

A tied interface can be used to connect two non-conforming meshes [40]. A tied interface requires the definition of both a primary and a secondary surface. It is assumed that the nodes of the primary surface are connected to the faces of the secondary surface. The following control parameters need to be defined:

<penalty>	penalty factor
<tolerance>	augmentation tolerance

3.13.6 Tied Elastic Interfaces

A tied elastic interface is similar to the tied interface. It may be used for tying solid materials. It enforces continuity of the displacement across the interface. The following control parameters need to be defined:

Parameter	Description	Default
penalty	normal penalty scale factor (1)	1.0
pressure_penalty	pressure penalty scale factor	1.0
auto_penalty	auto-penalty calculation flag (2)	0
update_penalty	update auto-penalty calculation flag (2)	0
two_pass	two-pass flag (3)	0
laugon	augmented Lagrangian flag (4)	0
tolerance	aug. Lagrangian convergence tolerance (4)	1.0
gaptol	tolerance for gap value (4)	0.0 (off)
symmetric_stiffness	symmetric stiffness matrix flag (7)	0
search_tol	Projection search tolerance (8)	0.01
search_radius	search radius (10)	1.0

3.13.7 Tied Biphasic Interfaces

A tied biphasic interface is similar to the tied interface. It may be used for tying any combination of solid, biphasic, and rigid materials. It enforces continuity of the fluid pressure across the interface when both materials are biphasic. The following control parameters need to be defined:

Parameter	Description	Default
penalty	normal penalty scale factor (1)	1.0
pressure_penalty	pressure penalty scale factor	1.0
auto_penalty	auto-penalty calculation flag (2)	0
update_penalty	update auto-penalty calculation flag (2)	0
two_pass	two-pass flag (3)	0
laugon	augmented Lagrangian flag (4)	0
tolerance	aug. Lagrangian convergence tolerance (4)	1.0
gaptol	tolerance for gap value (4)	0.0 (off)
symmetric_stiffness	symmetric stiffness matrix flag (7)	0
search_tol	Projection search tolerance (8)	0.01
search_radius	search radius (10)	1.0

3.13.8 Tied Multiphasic Interfaces

A tied multiphasic interface is similar to the tied biphasic interface. It may be used for tying any combination of solid, biphasic, multiphasic and rigid materials. It enforces continuity of the effective fluid pressure and effective solute concentrations across the interface when both materials are biphasic or multiphasic. The following control parameters need to be defined:

Parameter	Description	Default
penalty	normal penalty scale factor (1)	1.0
pressure_penalty	pressure penalty scale factor	1.0
concentration_penalty	concentration penalty scale factor	1.0
auto_penalty	auto-penalty calculation flag (2)	0
update_penalty	update auto-penalty calculation flag (2)	0
two_pass	two-pass flag (3)	0
laugon	augmented Lagrangian flag (4)	0
tolerance	aug. Lagrangian convergence tolerance (4)	1.0
gaptol	tolerance for gap value (4)	0.0 (off)
symmetric_stiffness	symmetric stiffness matrix flag (7)	0
search_tol	Projection search tolerance (8)	0.01
search_radius	search radius (10)	1.0

3.13.9 Sticky Interfaces

A sticky interface is similar to a tied interface except that it allows for initial separation of the tied surfaces and breaking of the tie after a user-defined normal traction is exceeded. The tie is only applied when the surfaces contact and sustained as long as the normal traction is less than the threshold.

Parameter	Description
laugon	augmentation flag
penalty	penalty factor
tolerance	augmentation tolerance
minaug	minimum number of required augmentations
maxaug	maximum number of augmentations
search_tolerance	tolerance for nodal projection onto secondary surface facet
max_traction	threshold for normal traction (1)
snap_tol	minimum distance for tie activation (2)

The contact surfaces are defined as in the *tied* interface (see Section 3.13.5).
Comments:

1. The *max_traction* parameter can be used to break the tied interface after the normal traction exceeds the specified value. Initially, this value is set to zero, in which case FEBio will ignore this value and the tie cannot be broken.

2. The *snap_tol* parameter is used in determining the minimum distance that a primary surface node must have approached the secondary surface facet in order to snap onto the secondary surface. The initial value is zero, meaning a node must have penetrated the secondary surface before it will be tied to it.

3.14 Constraints Section

The Constraints section allows the user to enforce additional constraints to the model.

3.14.1 Rigid Joints

Rigid joints produce nonlinear constraints between rigid bodies, which prevent relative motion except along the degrees of freedom of the joint. The term 'rigid' refers to the bodies, not to the joints. Each rigid joint needs to define two rigid bodies (a and b), a joint origin common to both bodies, and a set of axes that determine the relative orientation of the joint degrees of freedom. These axes define orthonormal basis vectors $\{\mathbf{e}_1^a, \mathbf{e}_2^a, \mathbf{e}_3^a\}$ and $\{\mathbf{e}_1^b, \mathbf{e}_2^b, \mathbf{e}_3^b\}$ on each rigid body, with both bases being coincident, $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, at the start of the analysis, and given in world coordinates.

The rigid joint nonlinear constraints produce reaction forces and moments that are enforced with penalty parameters and Lagrange multipliers. The penalty parameters, *force_penalty* and *moment_penalty*, may be conceptualized as stiffnesses of linear/torsional springs that prevent relative translations/rotations of the rigid bodies along degrees of freedom that must remain constrained for that joint. The penalty values should be selected based on a rough estimation of the maximum reactions forces and moments acting at these joints, divided by the maximum amount of linear/angular separation that your analysis can tolerate for that joint. Alternatively, set the *force_penalty* and *moment_penalty* parameters to 1 and turn on the *auto_penalty*; this setting will automatically adjust the *force_penalty* and *moment_penalty* to an appropriate value.

The augmented Lagrangian method is used by default, where the joint reaction force and moment are treated as Lagrange multipliers, augmented at each time step by the product of the force/moment penalty parameter and the linear/angular gap. Use the parameter *maxaug* to control the maximum allowable number of augmentations at each time step (*maxaug*=0 produces the penalty method); use a non-zero value for the parameter *minaug* to ensure a minimum number of augmentations. Augmentations will proceed until the relative change in the reaction force/moment magnitude is less than *tolerance*, and/or the linear gap is less than *gaptol*, and/or the angular gap is less than *angtol*. Setting any of these parameters to zero disables that check.

The nonlinear constraints that enforce these joints produce a non-symmetric stiffness matrix. Therefore, when using rigid joints, use the analysis setting for a non-symmetric formulation, see Section 3.3.4.

3.14.1.1 Rigid Revolute Joint

A rigid revolute joint connects rigid bodies a and b at a point in space, allowing one degree of freedom for rotation about an axis through that point:

```
<constraint type="rigid revolute joint" name="Joint 1">
  <tolerance>0</tolerance>
  <gaptol>1e-4</gaptol>
  <angtol>1e-4</angtol>
  <force_penalty>1e0</force_penalty>
  <moment_penalty>1e0</moment_penalty>
  <auto_penalty>1</auto_penalty>
  <body_a>1</body_a>
  <body_b>3</body_b>
```

```
  <joint_origin>-150,0,2</joint_origin>
  <rotation_axis>0,0,1</rotation_axis>
</constraint>
```

The *tolerance* element defines the augmentation tolerance. That is, when the relative change in the constraint forces and moments (the Lagrange multipliers) are less than this value. The *gaptol* element defines the tolerance for spatial separation of the joint origin on the two bodies (in units of length). The *angtol* element defines the tolerance for angular separation of the joint axis on the two bodies (in units of radians). Setting any of these three elements to zero disables the enforcement of that tolerance. The *force_penalty* parameter (with units of force per length) represents the stiffness that prevents the joint origin on the two bodies from separating. The *moment_penalty* parameter (with units of moment per radians) represents the torsional stiffness that enforces parallelism of the joint axis on the two bodies. The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *joint_origin* element defines the position of the joint origin (the origin of the basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$) in world coordinates at the start of the analysis. Note that this point does not have to be inside or on the surface of either of the two bodies. The *rotation_axis* element defines the orientation of the joint rotation axis $\mathbf{e}_1$ in world coordinates at the start of the analysis.

Optionally, the rotation of body b relative to body a may be prescribed using the additional tags

```
<prescribed_rotation>1</prescribed_rotation>
<rotation lc="1">3.14159</rotation>
```

The *prescribed_rotation* element is a flag that indicates that the motion of the joint is prescribed (1 for prescribed, 0 for free). The *rotation* element specifies the amount of rotation (with units of radians) with an optional associated load curve.

Optionally, a moment may be prescribed on body b relative to body a, about the joint axis, using the additional tag

```
<moment lc="1">5.e-3</moment>
```

The *moment* element specifies the magnitude of the moment, with an optional associated load curve. The *moment* element should not be used simultaneously with a prescribed rotation.

3.14.1.2 Rigid Prismatic Joint

A rigid prismatic joint connects rigid bodies a and b at a point in space, allowing one degree of freedom for translation along an axis through that point:

```
<constraint type="rigid prismatic joint" name="Joint02 ">
  <tolerance>0</tolerance>
  <gaptol>1e-4</gaptol>
  <angtol>1e-4</angtol>
  <force_penalty>1e0</force_penalty>
  <moment_penalty>1e0</moment_penalty>
  <auto_penalty>1</auto_penalty>
  <body_a>4</body_a>
  <body_b>1</body_b>
  <joint_origin>-150,0,2</joint_origin>
```

```
  <translation_axis>1,0,0</translation_axis>
  <prescribed_translation>150</prescribed_translation>
  <translation lc="1">1</translation>
</constraint>
```

The *tolerance* element defines the augmentation tolerance. That is, when the relative change in the constraint forces and moments (the Lagrange multipliers) are less than this value. The *gaptol* element defines the tolerance for spatial separation of the joint origin on the two bodies (in units of length). The *angtol* element defines the tolerance for angular separation of the joint axis on the two bodies (in units of radians). Setting any of these three elements to zero disables the enforcement of that tolerance. The *force_penalty* parameter (with units of force per length) represents the stiffness that prevents the joint origin on the two bodies from separating. The *moment_penalty* parameter (with units of moment per radians) represents the torsional stiffness that enforces parallelism of the joint axis on the two bodies. The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *joint_origin* element defines the position of the joint (the origin of the basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$) in world coordinates at the start of the analysis. Note that this point does not have to be inside or on the surface of either of the two bodies. The *translation_axis* element defines the orientation $\mathbf{e}_1$ of the joint translation axis in world coordinates at the start of the analysis.

Optionally, the translation of body b relative to body a may be prescribed using the additional tags

```
<prescribed_translation>1</prescribed_translation>
<translation lc="1">5.0</translation>
```

The *prescribed_translation* element is a flag that indicates that the motion of the joint is prescribed (1 for prescribed, 0 for free). The *translation* element specifies the amount of translation (with units of length) with an optional associated load curve.

Optionally, a force may be prescribed on body b relative to body a, along the joint axis using the additional tag

```
<force lc="1">5.e-3</force>
```

The *force* element specifies the magnitude of the force, with an optional associated load curve. The *force* element should not be used simultaneously with a prescribed translation.

3.14.1.3 Rigid Cylindrical Joint

A rigid cylindrical joint connects rigid bodies a and b at a point in space, allowing one degree of freedom for rotation about an axis through that point, and another degree of freedom for translation along that axis:

```
<constraint type="rigid cylindrical joint" name="Joint03">
  <tolerance>0</tolerance>
  <gaptol>1e-4</gaptol>
  <angtol>1e-4</angtol>
  <force_penalty>1e0</force_penalty>
  <moment_penalty>1e0</moment_penalty>
  <auto_penalty>1</auto_penalty>
```

```
  <body_a>1</body_a>
  <body_b>2</body_b>
  <joint_origin>0,0,0</joint_origin>
  <joint_axis>0,0,1</joint_axis>
</constraint>
```

The *tolerance* element defines the augmentation tolerance. That is, when the relative change in the constraint forces and moments (the Lagrange multipliers) are less than this value. The *gaptol* element defines the tolerance for spatial separation of the joint origin on the two bodies (in units of length). The *angtol* element defines the tolerance for angular separation of the joint axis on the two bodies (in units of radians). Setting any of these three elements to zero disables the enforcement of that tolerance. The *force_penalty* parameter (with units of force per length) represents the stiffness that prevents the joint origin on the two bodies from separating. The *moment_penalty* parameter (with units of moment per radians) represents the torsional stiffness that enforces parallelism of the joint axis on the two bodies. The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *joint_origin* element defines the position of the joint (the origin of the basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$) in world coordinates at the start of the analysis. Note that this point does not have to be inside or on the surface of either of the two bodies. The *joint_axis* element defines the orientation $\mathbf{e}_1$ of the joint rotation and translation axis in world coordinates at the start of the analysis.

Optionally, the rotation of body b relative to body a may be prescribed using the additional tags

```
<prescribed_rotation>1</prescribed_rotation>
<rotation lc="1">1.570796327</rotation>
```

The *prescribed_rotation* element is a flag that indicates that the motion of the joint is prescribed (1 for prescribed, 0 for free). The *rotation* element specifies the amount of rotation (with units of radians) with an optional associated load curve.

Optionally, the translation of body b relative to body a may be prescribed using the additional tags

```
<prescribed_translation>1</prescribed_translation>
<translation lc="2">10.0</translation>
```

Optionally, a moment may be prescribed about the joint axis using the additional tag

```
<moment lc="1">5.e-3</moment>
```

The *moment* element specifies the magnitude of the moment, with an optional associated load curve. The *moment* element should not be used simultaneously with a prescribed rotation.

Optionally, a force may be prescribed along the joint axis using the additional tag

```
<force lc="1">2.0</force>
```

The *force* element specifies the magnitude of the force, with an optional associated load curve. The *force* element should not be used simultaneously with a prescribed translation.

3.14.1.4 Rigid Spherical Joint

A rigid spherical joint connects rigid bodies a and b at a point in space, allowing three degrees of freedom for rotation about that point:

```
<constraint type="rigid spherical joint" name="Joint01">
  <tolerance>0.1</tolerance>
  <gaptol>0</gaptol>
  <force_penalty>1e0</force_penalty>
  <auto_penalty>1</auto_penalty>
  <body_a>1</body_a>
  <body_b>2</body_b>
  <joint_origin>0,0,0</joint_origin>
</constraint>
```

The *tolerance* element defines the augmentation tolerance. That is, when the relative change in the constraint forces and moments (the Lagrange multipliers) are less than this value. The *gaptol* element defines the tolerance for spatial separation of the joint origin on the two bodies (in units of length). Setting either of these elements to zero disables the enforcement of that tolerance. The *force_penalty* parameter (with units of force per length) represents the stiffness that prevents the joint origin on the two bodies from separating. The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *joint_origin* element defines the position of the joint (the origin of the basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$) in world coordinates at the start of the analysis. Note that this point does not have to be inside or on the surface of either of the two bodies. The *rotation_axis* element defines the orientation of the joint rotation axis in world coordinates at the start of the analysis.

Optionally, the rotation of body b relative to body a may be prescribed using the additional tags

```
<moment_penalty>1e0</moment_penalty>
<prescribed_rotation>1</prescribed_rotation>
<rotation_x lc="1">1</rotation_x>
<rotation_y lc="2">1</rotation_y>
<rotation_z>0</rotation_z>
```

The *prescribed_rotation* element is a flag that indicates that the motion of the joint is prescribed (1 for prescribed, 0 for free). The *rotation_x*, *rotation_y* and *rotation_z* elements specify the components $(\theta_1, \theta_2, \theta_3)$ of rotation (with units of radians), with optional associated load curves. The rotation occurs about the axis directed along $\theta_1\mathbf{e}_1^a + \theta_2\mathbf{e}_2^a + \theta_3\mathbf{e}_3^a$, with a magnitude $\sqrt{\theta_1^2 + \theta_2^2 + \theta_3^2}$. Either all or none of the rotation components must be prescribed, since all rotation components are needed to define a rotation tensor. The *moment_penalty* parameter (with units of moment per radians) represents the torsional stiffness that enforces tracking of the prescribed rotations between the two bodies.

Optionally, moments may be prescribed on body b relative to body a, about the world coordinate axes, using the additional tag

```
<moment_x lc="3">1.e-3</moment_x>
<moment_y lc="4">3.e-3</moment_y>
<moment_z lc="5">2.e-3</moment_z>
```

The *moment* elements specify the components of the moment vector in world coordinates, with optional associated load curves. The *moment* elements should not be used simultaneously with a prescribed rotation.

3.14.1.5 Rigid Planar Joint

A rigid planar joint connects rigid bodies a and b, allowing one degree of freedom for rotation about the axis $\mathbf{e}_1$ through that point, and two degrees of freedom for translations in the plane perpendicular to that axis, along $\mathbf{e}_2^a$ and $\mathbf{e}_3^a$:

```
<constraint type="rigid planar joint" name="Joint01">
  <tolerance>0</tolerance>
  <gaptol>1e-4</gaptol>
  <angtol>1e-4</angtol>
  <force_penalty>1e0</force_penalty>
  <moment_penalty>1e0</moment_penalty>
  <auto_penalty>1</auto_penalty>
  <body_a>1</body_a>
  <body_b>2</body_b>
  <joint_origin>0,0,0</joint_origin>
  <rotation_axis>0,-0.5,0.8660254</rotation_axis>
  <translation_axis_1>1,0,0</translation_axis_1>
</constraint>
```

The *tolerance* element defines the augmentation tolerance. That is, when the relative change in the constraint forces and moments (the Lagrange multipliers) are less than this value. The *gaptol* element defines the tolerance for spatial separation of the joint origin on the two bodies (in units of length). The *angtol* element defines the tolerance for angular separation of the joint axes on the two bodies (in units of radians). Setting any of these three elements to zero disables the enforcement of that tolerance. The *force_penalty* parameter (with units of force per length) represents the stiffness that prevents the joint origin on the two bodies from separating along the rotation axis. The *moment_penalty* parameter (with units of moment per radians) represents the torsional stiffness that enforces parallelism of the joint rotation axis on the two bodies. The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *joint_origin* element defines the position of the joint (the origin of the basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$) in world coordinates at the start of the analysis. Note that this point does not have to be inside or on the surface of either of the two bodies. The *rotation_axis* element defines the orientation of the joint rotation axis $\mathbf{e}_1$ in world coordinates at the start of the analysis. The *translation_axis_1* element defines the orientation of the joint translation axis $\mathbf{e}_2^a$ in the plane perpendicular to the joint rotation axis, in world coordinates at the start of the analysis.

Optionally, the rotation of body b relative to body a may be prescribed using the additional tags

```
<prescribed_rotation>1</prescribed_rotation>
<rotation lc="1">1.570796327</rotation>
```

The *prescribed_rotation* element is a flag that indicates that the motion of the joint is prescribed (1 for prescribed, 0 for free). The *rotation* element specifies the amount of rotation (with units of radians) with an optional associated load curve.

Optionally, the translation of body b relative to body a may be prescribed along $\mathbf{e}_2^a$ using the additional tags

```
<prescribed_translation_1>1</prescribed_translation_1>
<translation_1 lc="2">10.0</translation_1>
```

Optionally, the translation of body b relative to body a may be prescribed along $\mathbf{e}_3^a$ using the additional tags

```
<prescribed_translation_2>1</prescribed_translation_2>
<translation_2 lc="2">10.0</translation_2>
```

3.14.1.6 Rigid Lock

A rigid lock connects rigid bodies a and b, preventing relative motion between them. It requires the specification of a joint origin and two orthgonal axes $\mathbf{e}_1$ and $\mathbf{e}_2$:

```
<constraint type="rigid lock" name="Joint01">
  <tolerance>0</tolerance>
  <gaptol>1e-4</gaptol>
  <angtol>1e-4</angtol>
  <force_penalty>1e0</force_penalty>
  <moment_penalty>1e0</moment_penalty>
  <auto_penalty>1</auto_penalty>
  <body_a>1</body_a>
  <body_b>2</body_b>
  <joint_origin>0,0,0</joint_origin>
  <first_axis>1,0,0</first_axis>
  <second_axis>0,1,0</second_axis>
</constraint>
```

The *tolerance* element defines the augmentation tolerance. That is, when the relative change in the constraint forces and moments (the Lagrange multipliers) are less than this value. The *gaptol* element defines the tolerance for spatial separation of the joint origin on the two bodies (in units of length). The *angtol* element defines the tolerance for angular separation of the joint axes on the two bodies (in units of radians). Setting any of these three elements to zero disables the enforcement of that tolerance. The *force_penalty* parameter (with units of force per length) represents the stiffness that prevents the joint origin on the two bodies from separating along the rotation axis. The *moment_penalty* parameter (with units of moment per radians) represents the torsional stiffness that enforces parallelism of the joint rotation axis on the two bodies. The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *joint_origin* element defines the position of the joint (the origin of the basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$) in world coordinates at the start of the analysis. Note that this point does not have to be inside or on the surface of either of the two bodies. The *first_axis* element defines the orientation of the axis $\mathbf{e}_1$ in world coordinates at the start of the analysis. The *second_axis* element defines the orientation of the second axis $\mathbf{e}_2$ in world coordinates at the start of the analysis.

<Constraints> <constraint type="[name of update rule]"> <!-- parameters go here --> </constraint> </Constraints>

3.14.2 Rigid Connectors

Rigid connectors produce forces between rigid bodies. The term 'rigid' refers to the bodies, not to the connectors.

3.14.2.1 Rigid Spring

A rigid spring connects rigid bodies a and b with a linear spring:

```
<constraint type="rigid spring">
  <body_a>1</body_a>
  <body_b>2</body_b>
  <insertion_a>0,0,1</insertion_a>
  <insertion_b>0,0,3</insertion_b>
  <k>1</k>
</constraint>
```

The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *insertion_a* element defines the position of the spring insertion point on rigid body a. The *insertion_b* element defines the position of the spring insertion point on rigid body b. The k element represents the spring stiffness (in units of force per length). The resting length of the spring is the distance between insertion points at the start of the analysis.

3.14.2.2 Rigid Damper

A rigid damper connects rigid bodies a and b with a linear damper:

```
<constraint type="rigid damper">
  <body_a>1</body_a>
  <body_b>2</body_b>
  <insertion_a>0,0,1</insertion_a>
  <insertion_b>0,0,3</insertion_b>
  <c>1e-7</c>
</constraint>
```

The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *insertion_a* element defines the position of the damper insertion point on rigid body a. The *insertion_b* element defines the position of the damper insertion point on rigid body b. The c element represents the damping coefficient (in units of force per velocity).

3.14.2.3 Rigid Angular Damper

A rigid angular damper connects rigid bodies a and b with an angular damper:

```
<constraint type="rigid angular damper">
  <body_a>1</body_a>
  <body_b>2</body_b>
  <c>1e-3</c>
</constraint>
```

The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The c element represents the damping coefficient (in units of moment per angular velocity).

3.14.2.4 Rigid Contractile Force

A rigid contractile force connects rigid bodies a and b with a force actuator:

```
<constraint type="rigid contractile force">
  <body_a>1</body_a>
  <body_b>2</body_b>
  <insertion_a>0,0,1</insertion_a>
  <insertion_b>0,0,3</insertion_b>
  <f0 lc=''1''>1</f0>
</constraint>
```

The *body_a* and *body_b* elements are the material numbers of the two rigid bodies. The *insertion_a* element defines the position of the force actuator insertion point on rigid body a. The *insertion_b* element defines the position of the force actuator insertion point on rigid body b. The $f0$ element represents the actuator force (positive for contraction). Optionally, it may be associated with a load curve.

3.14.3 Symmetry Plane

A symmetry plane enforces zero solid displacement normal to a user-selected plane. This constraint is prescribed on a deformable surface of the model and is enforced for every node on that surface. It is the user's responsibility to select only planar surfaces.

```
<constraint type="symmetry plane" surface="SymmetryPlane01">
<laugon>1</laugon>
<penalty>1e6</penalty>
<tol>1e-6</tol>
<minaug>0</minaug>
<maxaug>50</maxaug>
</constraint>
```

The *surface* (SymmetryPlane01 in this example), is defined in the *Mesh* section. Let $\mathbf{u}$ denote the nodal displacement vector and let $\mathbf{n}$ denote the unit normal to the plane; the symmetry plane constraint enforces $u_n \equiv \mathbf{u}\cdot\mathbf{n} = 0$ using a penalty method, optionally with augmented Lagrangian. The reaction force needed to enforce this constraint is evaluated as εu_n, where ε is the user-specified *penalty* parameter (with units of force per length). To use the augmented Lagrangian method, set *laugon* to 1, and the Lagrange multiplier λ will be augmented as $\lambda \leftarrow \lambda + \varepsilon u_n$. Augmentations terminate when the relative change in λ is less than the user-specified tolerance *tol*, or when the number of augmentations exceeds *maxaug*.

3.14.4 Normal Fluid Velocity Constraint

A normal fluid velocity constraint forces the fluid velocity to remain normal to the selected surface. It is enforced for every node on that surface.

```
<constraint type="normal fluid velocity" surface="NormalFlowSurface01">
<laugon>1</laugon>
<penalty>1e6</penalty>
<tol>1e-6</tol>
<minaug>0</minaug>
<maxaug>50</maxaug>
</constraint>
```

The *surface* (NormalFlowSurface01 in this example), is defined in the *Mesh* section. Let $\mathbf{v}$ denote the nodal fluid velocity vector and let $\mathbf{n}$ denote the unit normal at each node; the normal flow constraint enforces $\mathbf{v} = (\mathbf{v}\cdot\mathbf{n})\,\mathbf{n}$, or equivalently, $\mathbf{v}_\tau = (\mathbf{I} - \mathbf{n}\otimes\mathbf{n})\cdot\mathbf{v} = \mathbf{0}$, using a penalty method, optionally with augmented Lagrangian. The reaction force needed to enforce this constraint is evaluated as $\varepsilon\mathbf{v}_\tau$, where ε is the user-specified *penalty* parameter (with units of force per velocity). To use the augmented Lagrangian method, set *laugon* to 1, and the vectorial Lagrange multiplier $\boldsymbol{\lambda}$ will be augmented as $\boldsymbol{\lambda} \leftarrow \boldsymbol{\lambda} + \varepsilon\mathbf{v}_\tau$. Augmentations terminate when the relative change in $\boldsymbol{\lambda}$ is less than the user-specified tolerance *tol*, or when the number of augmentations exceeds *maxaug*.

This constraint should only be used on a surface where the fluid dilatation has been fixed or prescribed. It is not compatible with boundary conditions that prescribe the fluid velocity. To prescribe a fluid velocity that remains normal to the selected surface, use the surface load *fluid normal velocity* (Section 3.12.2.12).

3.14.5 The Prestrain Update Rules

The prestrain update rules for are implemented via non-linear constraints in FEBio. This is done because non-linear constraints automatically participate in FEBio's augmentation mechanism, which allows the user to update and rerun the time step. The following section details how to setup the update rules in the FEBio input file and discusses the currently supported rules.

3.14.5.1 Using Update rules

In order to apply an update rule, a constraint definition must be added to the Constraints section of the input file. The type attribute is used to specify which update rule to use.

```
<Constraints>
  <constraint type="[name of update rule]">
    <!-- parameters go here -->
  </constraint>
</Constraints>
```

The following table lists the available update rules.

type	description
prestrain	Eliminate distortion due to incompatibility
in-situ stretch	Enforce the given in-situ fiber stretches

Below, the supported update rules are presented in more detail. All of them share parameters for controlling the convergence of the update algorithm and these shared parameters are listed in the following table.

parameter	description	initial value
update	update flag (1)	1
tolerance	convergence tolerance	0.0
min_iters	minimum number of iterations	0
max_iters	maximum number of iterations	-1 (i.e. ignored)

Comments:

1. By specifying a loadcurve for the update flag, the update can be delayed. This can be useful if, for instance, the prestrain is applied incrementally and the update rule should not be applied until the full prestrain field is applied. In that case, specifying a loadcurve for the update flag that is zero while the prestrain is applied, will delay the update process.

3.14.5.2 prestrain update rule

The idea behind this rule is to eliminate the distortion induced by the incompatibility of the initial prestrain gradient with the reference geometry. Thus, we retain the original reference geometry at the cost of an altered effective prestain field. The update rule is given by the following equation.

$$\mathbf{G}^{k+1} = \mathbf{G}^{k} \cdot \mathbf{F}_{c} \tag{3.14.1}$$

This update rule does not define any additional parameters aside the ones from above.
Example:

```
<constraint type="prestrain">
  <tolerance>0.01</tolerance>
</constraint>
```

3.14.5.3 The in-situ stretch update rule

The idea behind this update rule is to enforce the fiber stretch induced by the initial prestrain gradient. As with the in-situ stretch generator option, this rule has an isochoric version and an uniaxial version for the update rule.

$$\mathbf{G}_{iso} = \mathbf{Q}\begin{bmatrix} \lambda^{-1} & & \\ & \lambda^{1/2} & \\ & & \lambda^{1/2} \end{bmatrix}\mathbf{Q}^T, \qquad \mathbf{G}_{uni} = \mathbf{Q}\begin{bmatrix} \lambda^{-1} & & \\ & 1 & \\ & & 1 \end{bmatrix}\mathbf{Q}^T \tag{3.14.2}$$

where $\lambda^2 = \mathbf{a}_0 \cdot \mathbf{C}^k \cdot \mathbf{a}_0$, is the fiber stretch induced by the distortion.

parameter	description	initial value
isochoric	Choose the isochoric update rule or not	1(=true)

Example:

```
<constraint type="in-situ stretch">
  <tolerance>0.01</tolerance>
  <isochoric>1</isochoric>
</constraint>
```

3.15 Discrete Section

This section defines the materials used by the discrete elements and assigns these materials to the discrete elements sets defined in the *Mesh* section. The materials are defined via the *discrete_material* element and the materials are assigned to discrete element sets using the *discrete* element.

```
<Discrete>
  <discrete_material id="1" type="nonlinear spring">
    <force lc="1">1.0</force>
  </discrete_material>
  <discrete_material id="2" type="linear spring">
    <E>2.0</E>
  </discrete_material>
  <discrete dmat="1" discrete_set="springs1"/>
  <discrete dmat="2" discrete_set="springs2">
</Discrete>
```

The *discrete_material* and the *discrete* elemens are defined in more detail below.

3.15.1 Discrete Materials

The *discrete_material* section defines a material that can be assigned to a discrete element set. The *id* attribute defines the material ID and the *type* attribute defines the material type. The following types are currently supported.

Type	Description
linear spring	spring that has a linear force-displacement relation
nonlinear spring	user defines the force-displacement relation

The linear element requires the E parameter that defines the spring constant.

The nonlinear spring requires the *force* parameter which defines the loadcurve that will be used for the force-displacement relation.

3.15.2 Discrete Section

After the discrete materials are defined, the materials are assigned to the discrete element sets that are defined in the *Mesh* section using the *discrete* element. This element requires two attributes:

dmat discrete material ID

discrete_set discrete element set defined in the *Mesh* section

3.15.3 Rigid Cable

A rigid cable can be used to apply a load to a series of rigid bodies that are connected at fixed points (fixed with respect to the rigid body). The cable runs through these points and the user can prescribe the force at the end of the cable. The rigid cable requires the following parameters.

force The magnitude of the force applied at the end of the cable.

force_direction The direction of the force (FEBio will normalize this vector if needed.)

relative If set to 1 the coordinates of the fixed points are relative to the rigid body frame of reference, otherwise they are in global coordinates.

point For each fixed point, enter the coordinates of the point. This tag requires the rb attribute to denote the rigid body it is attached to.

The following shows an example.

```
<rigid_cable>

    <force lc="1">1000</force>
    <force_direction>0,0,-1</force_direction>
    <relative>1</relative>
    <point rb="1">0,0,0</point>
    <point rb="2">0,0,0</point>

</rigid_cable>
```

This example defines a cable that runs through the centers of mass of two rigid bodies. The force is applied in the -z direction at the end of the cable (i.e. point 2).

3.16 LoadData Section

The *LoadData* section is used to define load controllers. A load controller allows users to manipulate the value of most model parameters as an explicit or implicit function of time. Use the *type* attribute to define a particular controller. Currently the following load controllers are available:

- **loadcurve**: the controller is a load curve, which is a tabulated list of time-value pairs. The user can set how the points are interpolated and how to extend the curve outside of its specified interval.
- **math**: the math controller allows the user to specify a mathematical expression that defines a function of time. Other model parameters can be used in the mathematical expression.
- **PID**: a PID controller.

3.16.1 The loadcurve controller

A loadcurve controller is defined by the *loadcurve* type. Each loadcurve is defined by repeating the *point* element for all data points:

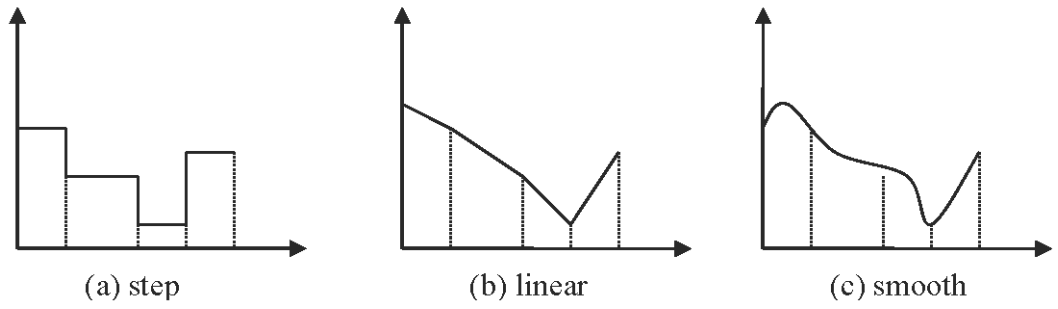
```
<load_controller id="1" [interpolate="type" extend="extend"]>
  <point> 0, 0 </point>
  ...
  <point> 1, 1 </point>
</loadcurve>
```

For a loadcurve, the type is optional, since it is the default controller if the type attribute is omitted.

The *id* attribute is the loadcurve number and is used in other sections of the input file as a means to reference this curve.

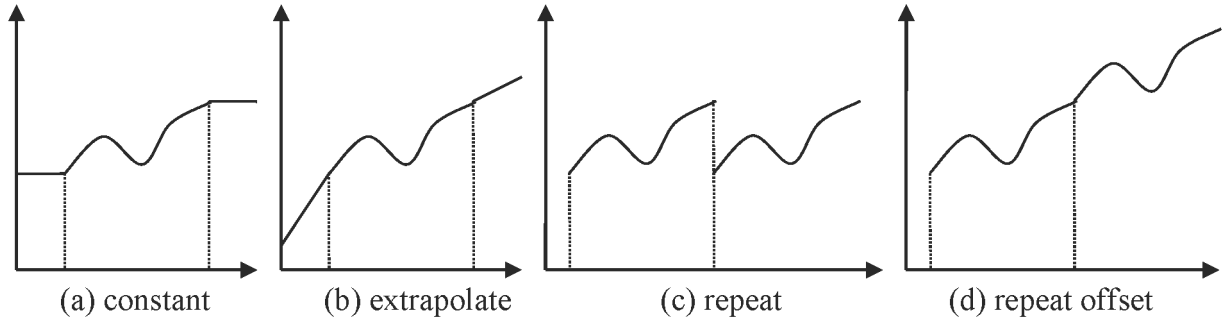
The optional attributes *interpolate* and *extend* define how the value of the loadcurve is interpolated from the data points. The interpolate defines the interpolation function and *extend* defines how the values of the loadcurve are determined outside of the interval defined by the first and last data point. The following tables list the possible values. The default values are marked with an asterisk (*).

interpolate	Description
step	Use a step interpolation function
linear*	Use a linear interpolation function
smooth	The values are interpolated using a cubic spline.



The different values for the *type* attribute of load curves

Extend	Description
constant	The value of the curve is the value of the closest endpoint
extrapolate*	The value is extrapolated linearly from the endpoints
repeat	The curve is repeated
repeat offset	The curve is repeated but offset from the endpoints



The different values for the *extend* attribute of the load curve.

3.16.2 The math controller

Use the “math” value for the *type* attribute to define a math controller. This controller allows users to use a mathematical expression that defines a function of time. Use the “t” parameter to reference time.

```
<load_controller id="1" type="math">
    <math>2.0*sin(pi*t)</math>
</load_controller>
```

3.16.3 The PID controller

The PID controller allows users to create simple control systems where the value of one model parameter is used to control the output of another model parameter. The PID controller calculates the output value as a sum of three terms: a term proportional to the error (i.e. the difference between a user-defined target value and the measurement), a derivative term, and an integral term.

This controller requires the following parameters:

- **var**: specify the model parameter that is used as process variable, i.e. the measurement.
- **target**: the target value for the process variable.
- **Kp**: weight factor for the proportional term.
- **Kd**: weight factor for the derivative term
- **Ki**: weight factor for the integral term.

For example:

```
<load_controller id="1" type="PID">
    <var>fem.rigid_body[1].euler.z</var>
    <target>1.5708</target>
    <Kp>5</Kp>
    <Kd>1</Kd>
    <Ki>4</Ki>
</load_controller>
```

3.17 Output Section

FEBio usually splits the output in two files: the *logfile,* which contains the same information that was written to the screen during the analysis, and the *plotfile,* which contains the results. The contents of these output files can be customized in the *Output* section.

3.17.1 Logfile

The logfile records the same output that is printed to the screen. In addition, the user can request FEBio to output additional data to the logfile. This feature is called *data logging*. To use this feature, simply define the following element in the *Output* section of the input file:

```
<Output>
  <logfile [file="<log file>"]>
    <node_data [attributes]>item list</node_data>
    <element_data [attributes]>item list</element_data>
    <rigid_body_data [attributes]>item list</rigid_body_data>
  </logfile>
</Output>
```

The optional attribute *file* defines the name of the logfile. If omitted, a default name is used that is derived from the FEBio input file. See Section 2.7 for details on default naming conventions for output files.

Additional data is stored to the logfile by adding one or more of the following elements:

node_data request nodal data

element_data request element data

rigid_body_data request rigid body data

Each of these data classes takes the following attributes:

data an expression defining the data that is to be stored

name a descriptive name for the data (optional; default = data expression)

file the name of the output file where the data is stored. (optional; default = logfile)

delim the delimiter used to separate data in multi-column format (optional; default = space)

format an optional format string (optional; default = not used)

The *data* attribute is the most important one and is mandatory. It contains a list of variable names, separated by a semi-colon. The available variable names depend on the data class and are defined below. For example, the data expression:

```
data="x;y;z"
```

will store the variables x, y and z in separate columns. See below for more examples.

The optional *name* attribute is a descriptive name for the data. It is used in the logfile to refer to this data and can be used to quickly find the data record in the logfile. If omitted, the data expression is used as the name.

The *file* attribute defines the name of the output file where the data is to be stored. This attribute is optional and when not specified the data will be stored in the logfile.

The optional *delim* attribute defines the delimiter that is used in multi-column format. As described above, data can be stored in multiple columns and the delimiter is used to separate the columns. The default is a single space.

The optional *format* attribute defines a format string that will be used to format the output. If this attribute is present, the *delim* attribute will be ignored. The format string is composed of literal characters and special formatting characters. The special formatting characters are preceded by the percentage character (%). The following formatting characters are currently defined.

%i replace with the index of the corresponding item (i.e. node numbers for node data)

%g replace with a data value. Use a %g for each data item.

%t insert tab character in output.

%n insert newline character in output.

The following example,

```
<node_data data="x;y;z" format='<node id="%i">%g,%g,%g</node>'></node_data>
```

will print the following output (e.g. for node 1).

```
<node id="1">0.1,0.2,0.3</node>
```

Notice the use of the apostrophe (') in the format string. This is necessary in order to include the quotation marks as part of the format string. Also note that each data string will automatically be printed on a new line, so there is no need to end the format string with a newline character.

The value of the data elements is a list of items for which the data is to be stored. For example, for the *node_data* element the value is a list of nodes, for the *element_data* element it is a list of FE elements and for the *rigid_body* element it is a list of rigid bodies. The value may be omitted in which case the data for all items will be stored. For instance, omitting the value for the *node_data* element will store the data for all nodes.

As stated above, the data is either stored in the logfile or in a separate file. In any case, a record is made in the logfile. When storing the data in the logfile, the following entry will be found in the logfile at the end of each converged timestep for each data element:

```
Data Record #<n>
Step = <time step>
Time = <time value>
Data = <data name>
<actual data goes here>
```

The record number n corresponds to the nth data element in the input file. The *Step* value is the current time step. The *Time* value is the current solution time. The *Data* value is the name of the data element as provided by the *name* attribute (or the *data* attribute if *name* is omitted). The actual data immediately follows this record. If multiple column output is used, the columns are separated by the *delim* attribute of the data element.

When storing the data in a separate file, the format is slightly different:

```
Data Record #<n>
Step = <time step>
Time = <time value>
Data = <data name>
File = <file name>
```

The *File* value is the name of the physical file. Note that this is the name to which the time step number is appended. In addition, the physical file that stores the data contains the following header:

```
*Title = <problem title>
*Step = <time step>
*Time = <time value>
*Data = <data name>
<actual data goes here>
```

The problem title is as defined in the input file.

In either case, the actual data is a multi-column list, separated by the delimiter specified with the *delim* attribute (or a space when omitted). The first column always contains the item number. For example, the following data element:

```
<node_data
data="x;y;z" name="nodal coordinates" delim=",">1:4:1</node_data>
```

will result in the following record in the logfile:

```
Data Record #1
Step = 1
Time = 0.1
Data = "nodal coordinates"
1,0.000,0.000,0.000
2,1.000,0.000,0.000
3,1.000,1.000,0.000
4,0.000,1.000,0.000
```

This data record is repeated for each converged time step. The following sections define the data variables that are available for each of the data classes.

3.17.1.1 Node_Data Class

The *node_data* class defines a set of nodal variables. The data is stored for each node that is listed in the item list of the *node_data* element or for all nodes if no list is defined. The following nodal variables are defined.

Node variables	Description
x	x-coordinate of current nodal position
y	y-coordinate of current nodal position
z	z-coordinate of current nodal position
ux	x-coordinate of nodal displacement
uy	y-coordinate of nodal displacement
uz	z-coordinate of nodal displacement
vx	x-coordinate of nodal velocity
vy	y-coordinate of nodal velocity
vz	z-coordinate of nodal velocity
ax	x-coordinate of nodal acceleration
ay	y-coordinate of nodal acceleration
az	z-coordinate of nodal acceleration
Rx	x-coordinate of nodal reaction force
Ry	y-coordinate of nodal reaction force
Rz	z-coordinate of nodal reaction force

For analyses using biphasic, biphasic-solute, and triphasic materials, the following additional variables can be defined.

Node variables	Description
p	effective fluid pressure
vx	x-component of solid velocity
vy	y-component of solid velocity
vz	z-component of solid velocity
c[n]	effective concentration of solute n, with n from 1 to 8

For heat transfer problems the following nodal variables are available.

Node variables	Description
T	Nodal temperature

For fluid analyses, the following variables can be defined.

Node variables	Description
vx	x-component of fluid velocity
vy	y-component of fluid velocity
vz	z-component of fluid velocity

For example, to store the current nodal positions of all nodes, use the following *node_data* element:

```
<node_data data="x;y;z"></node_data>
```

You can store the total nodal displacement for nodes 1 through 100, and all even numbered nodes 200 through 400 as follows:

```
<node_data data="ux;uy;uz">1:100:1,200:400:2</node_data>
```

3.17.1.2 Element_Data Class

The *element_data* class defines a set of element variables. The data is stored for each element that is listed in the item list of the *element_data* element or for all nodes if no list is defined. The following element variables are defined. Note that the actual value is the average over the element's integration points values (if applicable).

Element variables	Description
x	x-coordinate of current element centroid position
y	y-coordinate of current element centroid position
z	z-coordinate of current element centroid position
sx	xx-component of the Cauchy stress
sy	yy-component of the Cauchy stress
sz	zz-component of the Cauchy stress
sxy	xy-component of the Cauchy stress
syz	yz-component of the Cauchy stress
sxz	xz-component of the Cauchy stress
s1	first eigenvalue of Cauchy stress tensor
s2	second eigenvalue of Cauchy stress tensor
s3	third eigenvalue of Cauchy stress tensor
Ex	xx-component of the Green-Lagrange strain
Ey	yy-component of the Green-Lagrange strain
Ez	zz-component of the Green-Lagrange strain
Exy	xy-component of the Green-Lagrange strain
Eyz	yz-component of the Green-Lagrange strain
Exz	xz-component of the Green-Lagrange strain
E1	first eigenvalue of Green-Lagrange strain tensor
E2	second eigenvalue of Green-Lagrange strain tensor
E3	third eigenvalue of Green-Lagrange strain tensor
Fxx	xx-component of the deformation gradient
Fyy	yy-component of the deformation gradient
Fzz	zz-component of the deformation gradient
Fxy	xy-component of the deformation gradient
Fyz	yz-component of the deformation gradient
Fxz	xz-component of the deformation gradient
Fyx	yx-component of the deformation gradient
Fzy	zy-component of the deformation gradient
Fzx	xz-component of the deformation gradient
J	relative volume (determinant of deformation gradient)
cxxxx	xxxx component of spatial elasticity tensor (a.k.a. c11)
cxxyy	xxyy component of spatial elasticity tensor (a.k.a. c12)
cyyyy	yyyy component of spatial elasticity tensor (a.k.a. c22)
cxxzz	xxzz component of spatial elasticity tensor (a.k.a. c13)
cyyzz	yyzz component of spatial elasticity tensor (a.k.a. c23)
czzzz	zzzz component of spatial elasticity tensor (a.k.a. c33)
cxxxy	xxxy component of spatial elasticity tensor (a.k.a. c14)

cyyxy	yyxy component of spatial elasticity tensor (a.k.a. c24)
czzxy	zzxy component of spatial elasticity tensor (a.k.a. c34)
cxyxy	xyxy component of spatial elasticity tensor (a.k.a. c44)
cxxyz	xxyz component of spatial elasticity tensor (a.k.a. c15)
cyyyz	yyyz component of spatial elasticity tensor (a.k.a. c25)
czzyz	zzyz component of spatial elasticity tensor (a.k.a. c35)
cxyyz	xyyz component of spatial elasticity tensor (a.k.a. c45)
cyzyz	yzyz component of spatial elasticity tensor (a.k.a. c55)
cxxxz	xxxz component of spatial elasticity tensor (a.k.a. c16)
cyyxz	yyxz component of spatial elasticity tensor (a.k.a. c26)
czzxz	zzxz component of spatial elasticity tensor (a.k.a. c36)
cxyxz	xyxz component of spatial elasticity tensor (a.k.a. c46)
cyzyz	yzyz component of spatial elasticity tensor (a.k.a. c56)
cxzxz	xzxz component of spatial elasticity tensor (a.k.a. c66)
sed	strain energy density
devsed	deviatoric strain energy density
D	damage variable (or sum of damage variables in solid mixtures)

For analyses using biphasic, biphasic-solute, and triphasic materials, the following additional variables can be defined:

Element variables	**Description**
p	actual fluid pressure
cn	actual concentration of solute n
wx	x-component of fluid flux
wy	y-component of fluid flux
wz	z-component of fluid flux
jnx	x-component of flux of solute n
jny	y-component of flux of solute n
jnz	z-component of flux of solute n

For fluid analyses, the following additional variables can be defined:

Element variables	**Description**
fx	x-coordinate of element centroid position
fy	y-coordinate of element centroid position
fz	z--coordinate of element centroid position
fp	fluid pressure
fvx	x-component of fluid velocity
fvy	y-component of fluid velocity

fvz	z-component of fluid velocity
fJ	fluid volume ratio
fd	fluid density
fsp	fluid stress power
fax	x-component of fluid acceleration
fay	y-component of fluid acceleration
faz	z-component of fluid acceleration
fwx	x-component of fluid vorticity
fwy	y-component of fluid vorticity
fwz	z-component of fluid vorticity
fsxx	xx-component of fluid Cauchy stress
fsyy	yy-component of fluid Cauchy stress
fszz	zz-component of fluid Cauchy stress
fsxy	xy-component of fluid Cauchy stress
fsyz	yz-component of fluid Cauchy stress
fsxz	xz-component of fluid Cauchy stress
fdxx	xx-component of fluid rate of deformation
fdyy	yy-component of fluid rate of deformation
fdzz	zz-component of fluid rate of deformation
fdxy	xy-component of fluid rate of deformation
fdyz	yz-component of fluid rate of deformation
fdxz	xz-component of fluid rate of deformation

For example, to store the (average) Cauchy stress for all elements, define the following data element:

```
<element_data data="sx;sy;sz;sxy;syz;sxz" name="element stresses"> </element_data>
```

3.17.1.3 Rigid_Body_Data Class

The *rigid_body_data* class defines a set of variables for each rigid body. The data is stored for each rigid body that is listed in the item list of the *rigid_body_data* element or for all rigid bodies if no list is defined. The following variables are defined. Note that the item referenced in the item list is the material number of the rigid body.

Rigid body variables	**Description**
x	x-coordinate of center of mass position
y	y-coordinate of center of mass position
z	z-coordinate of center of mass position
vx	x-component of center of mass velocity
vy	y-component of center of mass velocity
vz	z-component of center of mass velocity

ax	x-component of center of mass acceleration
ay	y-component of center of mass acceleration
az	z-component of center of mass acceleration
thx	x-component of rotation pseudo-vector
thy	y-component of rotation pseudo-vector
thz	z-component of rotation pseudo-vector
omx	x-component of angular velocity
omy	y-component of angular velocity
omz	z-component of angular velocity
alx	x-component of angular acceleration
aly	y-component of angular acceleration
alz	z-component of angular acceleration
qx	x-component of rotation quaternion
qy	y-component of rotation quaternion
qz	z-component of rotation quaternion
qw	w-component of rotation quaternion
Fx	x-component of the rigid body reaction force
Fy	y-component of the rigid body reaction force
Fz	z-component of the rigid body reaction force
Mx	x-component of the rigid body reaction torque
My	y-component of the rigid body reaction torque
Mz	z-component of the rigid body reaction torque
KE	kinetic energy

For example, to store the rigid body reaction force of rigid body 2 and 4 add the following data element. Note that the 2 and 4 refer to the rigid body material number as defined in the *Material* section of the input file:

```
<rigid_body_data data="Fx;Fy;Fz">2,4</rigid_body_data>
```

3.17.1.4 Rigid_Connector_Data Class

The *rigid_connector_data* class defines a set of variables for each rigid joint or rigid connector. The data is stored for each rigid joint or rigid connector that is listed in the item list of the *rigid_connector_data* element or for all rigid connectors if no list is defined. The following variables are defined. Note that the item referenced in the item list is the rigid connector number in the order in which rigid connectors appear in the input file.

Rigid body variables	**Description**
RCFx	x-component of rigid connector force
RCFy	y-component of rigid connector force
RCFz	z-component of rigid connector force
RCMx	x-component of rigid connector moment

RCMy	y-component of rigid connector moment
RCMz	z-component of rigid connector moment
RCx	x-component of rigid connector translation
RCy	y-component of rigid connector translation
RCz	z-component of rigid connector translation
RCthx	x-component of rigid connector rotation
RCthy	y-component of rigid connector rotation
RCthz	z-component of rigid connector rotation

For example, to store the reaction forces and moments at rigid joints 2 and 4 add the following data element:

```
<rigid_connector_data data="RCFx;RCFy;RCFz;RCMx;RCMy;RCMz">2,4</rigid_connector_data>
```

The rigid connector translation and rotation variables return relative motions of the rigid bodies connected by rigid joints (Section 3.14.1) and other rigid connectors (Section 3.14.2). The rotation components represent the components of a vector whose direction is along the axis of rotation, and whose magnitude is the (counter-clockwise) angle of rotation. These relative motions are calculated as the motion of *body_b* relative to *body_a*, expressed in the local Cartesian basis of *body_a*, whose initial origin is at *joint_origin*. This Cartesian basis (which generally moves with *body_a*) has its first axis along *rotation_axis* (for revolute and planar joints) or *translation_axis* (for prismatic joints) or *joint_axis* (for cylindrical joints); the second axis is along the *transverse_axis* (for revolute, prismatic and cylindrical joints) or *translation_axis_1* (for planar joints). For spherical joints, springs, dampers, angular dampers and contractile forces, the axes are always aligned with the global Cartesian basis.

For springs, dampers and contractile forces, the returned translation components represent the relative position vector between insertion points on *body_b* and *body_a*. The magnitude of this vector represents the distance between those points.

3.17.2 Plotfile

By default, all the results are stored in a binary database, referred to as the *plotfile*. The preferred storage format is the FEBio bindary database format (referred to as the *xplt* format)[4]. This section describes how to customize the data that is stored in the *xplt* format.

To define the contents of the plotfile you need to define the *plotfile* element in the Output section of the FEBio input file.

```
<plotfile type="febio" [file="name.xplt"]/>
```

The *file* attribute is optional and allows the user to define the file name of the plotfile. If this attribute is omitted, FEBio will use a default file name for the plotfile.

By default, FEBio will store the most common data variables to the plot file. However, it is advised to always specify the specific contents of the plotfile. This can be done by adding *var* elements in the *plotfile* section.

[4] As of FEBio version 2.0, the LSDYNA database is no longer supported. The FEBio database format is the only format that will be supported from now on.

3.17.2.1 Plotfile Variables

Plotfile variables are defined using the *var* keyword. This tag takes one parameter, namely the *type* of the variable.

```
<var type="<name>"/>
```

where *name* is the name of the variable. The following table lists the possible values for *name*.

Name	Variable	Description
Acceleration	Element	Average element accelerations
contact area	Surface	Net contact area across contact interface. Evaluated by integrating the surface area at integration points where the contact pressure is not zero.
contact force	Surface	Net contact force across contact interface. Evaluated by integrating the contact traction over the contact surface.
contact gap	Surface	Contact gap distance, evaluated at contact surface faces
contact penalty	Surface	Contact penalty value
contact pressure	Surface	Contact pressure, evaluated at contact surface faces
contact stick	Surface	Stick status in stick-slip frictional contact (1=stick, 0=slip). Values between 0 and 1 imply that a fraction of that face is in stick mode. Currently works only with sliding-tension-compression.
contact traction	Surface	Contact traction vectors, evaluated at contact surface faces
current density	Element	Electric current density, Eq.(4.9.11)
current element angular momentum	Element	The element's total angular momentum at the current configuration.
current element center of mass	Element	The element's center of mass at the current configuration.
current element kinetic energy	Element	The element's total kinetic energy at the current configuration.
current element linear momentum	Element	The element's total linear momentum at the current configuration
current element strain energy		The element's total strain energy at the current configuration.
damage	Element	Damage variable D (Section 4.5)
density	Element	The current density
deviatoric strain energy density	Element	Deviatoric strain energy density $\tilde{\Psi}\left(\tilde{\mathbf{C}}\right)$, Eq.(4.1.1)
displacement	Node	Nodal displacements

effective elasticity	Element	The elasticity of the elastic material in a biphasic/triphasic/multiphasic material.
effective fluid pressure	Node	fluid pressure for biphasic, biphasic-solute, triphasic, and multiphasic materials.
effective shell fluid pressure	Node	fluid pressure for biphasic, biphasic-solute, triphasic, and multiphasic materials of shell domains.
effective shell solute concentration	Node	Effective solute concentration for biphasic-solute, triphasic, and multiphasic materials of shell domains.
effective solute concentration	Node	Effective solute concentration for biphasic-solute, triphasic, and multiphasic materials.
effective fluid pressure	Node	Fluid pressure p for biphasic materials, Eq.(4.7.1), or $\tilde{p}$ for biphasic-solute, Eq.(4.8.3) and triphasic/multiphasic materials, Eq.(4.9.7)
effective solute concentration	Node	Effective solute concentration $\tilde{c}$ for biphasic-solute materials, Eq.(4.8.3), and triphasic/multiphasic materials, Eq.(4.9.7)
elasticity	Element	Spatial elasticity tensor components
electric potential	Element	Electric potential ψ in triphasic/multiphasic materials, Section 4.9
element angular momentum	Element	Element total angular momentum
element center of mass	Element	Element center of mass
element kinetic energy	Element	Element total kinetic energy
element linear momentum	Element	Element total linear momentum
element strain energy	Element	Element total strain energy
element stress power	Element	Element total stress power
enclosed volume	Surface*	Volume enclosed by named surface
Euler angle	Rigid body	Rigid body Euler angles
fiber stretch	Element	Element's average fiber stretch
fiber vector	Element	Material fiber vector
fixed charge density	Element	Fixed charge density c^F in current configuration, Eq.(4.9.2)
fluid acceleration	Element	Fluid acceleration (material time derivative of fluid velocity $\mathbf{v}^f$, Section (4.13)
fluid density	Element	Fluid density ρ^f in fluid and fluid-FSI materials, Eq.(4.13.3)
fluid dilatation	Node	Fluid dilatation e, Section (4.13))
fluid element angular momentum	Element	Total angular momentum of fluid element
fluid element center of mass	Element	Center of mass of fluid element
fluid element kinetic energy	Element	Total kinetic energy of fluid element
fluid element linear momentum	Element	Total linear momentum of fluid element

fluid element strain energy	Element	Total strain energy of fluid element
fluid energy density	Element	Average energy density of fluid element
fluid flow rate	Surface*	Volumetric fluid flow rate $Q = \int_A \mathbf{w} \cdot \mathbf{n}\, dA$ across a named surface (biphasic and multiphasic analyses)
fluid flux	Element	Fluid flux $\mathbf{w}$ in biphasic, Eq.(4.7.2), biphasic-solute, Eq.(4.8.4), and triphasic/multiphasic materials, Eq.(4.9.9)
fluid force	Surface	Net fluid force across biphasic (sliding-biphasic), biphasic-solute (sliding-biphasic-solute) and multiphasic (sliding-multiphasic) contact interface. Evaluated by integrating the fluid pressure p over the contact surface.
fluid force2	Surface	Alternative calculation of the net fluid force
fluid heat supply density	Element	Average heat supply density of a fluid element
fluid kinetic energy density	Element	Average kinetic energy densify of a fluid element
fluid load support	Surface	The total fluid load support across a named surface
fluid mass flow rate	Surface*	Mass flow rate across a named surface, $\dot{m} = \int_A \rho \mathbf{v} \cdot \mathbf{n}\, dA$, Section (4.13)
fluid pressure	Element	Fluid pressure p in biphasic, Eq.(4.7.1), biphasic-solute, Eq.(4.8.3), triphasic/multiphasic materials, Eq.(4.9.7), and fluid materials, Eq.(4.13.2)
fluid rate of deformation	Element	Fluid rate of deformation tensor $\mathbf{D}$, Section (4.13)
fluid shear viscosity	Element	Average shear viscosity of a fluid element
fluid strain energy density	Element	Average shear energy density of fluid element
fluid stress	Element	Fluid stress $\boldsymbol{\sigma}$, Eq.(4.13.1)
fluid stress power density	Element	Fluid stress power $\boldsymbol{\sigma} : \mathbf{D}$, Section (4.13)
fluid surface energy flux	Surface	The total energy flux across a named surface for a fluid analysis
fluid surface force	Surface*	Net force exerted by a fluid on a named surface, $\mathbf{f} = -\int_A \mathbf{t}\, dA$, Section (4.13)
fluid surface pressure	Surface*	Average fluid pressure on each face of a surface, evaluated from the nodal values of the fluid dilatation on that face
fluid surface traction power	Surface	Net traction power across a named surface of a fluid analysis
fluid velocity	Element	Element fluid velocity $\mathbf{v}^f$ in fluid and fluid-FSI materials, Section (4.13)
fluid volume ratio	Element	Fluid volume ratio J, Section (4.13)

fluid vorticity	Element	Fluid vorticity, Section (4.13)
heat flux	Element	The average heat flux inside an element of a heat-transfer analysis
kinetic energy density	Element	The average kinetic energy density in an element
Lagrange strain	Element	The average Lagrange strain in an element
nested damage	Element	The average damage in an elastic mixture
nodal acceleration	Node	The acceleration at the nodes
nodal contact gap	Surface	Contact gap distance, evaluated at contact surface nodes
nodal contact pressure	Surface	Contact pressure, evaluated at contact surface nodes
nodal contact traction	Surface	Contact traction vectors, evaluated at contact surface nodes
nodal fluid flux	Element	Fluid flux in biphasic, biphasic-solute, triphasic, and multiphasic materials
nodal fluid velocity	Node	Fluid velocity $\mathbf{v}^f$ in fluid and fluid-FSI materials
nodal relative fluid velocity	Node	Fluid velocity relative to mesh $\mathbf{w}$ in fluid and fluid-FSI materials
nodal stress	Element	The Cauchy stress, projected to the nodes.
nodal surface traction	Surface	Contact nodal tractions
nodal vector gap	Surface	Contact gap vector at surface nodes
nodal velocity	Node	The nodal velocities
osmolarity	Element	Element's average osmolarity in biphasic/triphasic/multiphasic analysis
parameter	Element	Stores heterogeneous material parameter data
pressure gap	Surface	Pressure gap between opposing surfaces in a biphasic contact analysis
reaction forces	Node	The nodal reaction forces.
receptor-ligand concentration	Element	Receptor-ligand concentration in a biphasic-solute analysis.
referential fixed charge density	Element	Referential fixed charge density c_r^F, Eq.(4.9.2), which may evolve with chemical reactions, Eq.(4.10.10)
referential solid volume fraction	Element	Referential solid volume fraction φ_r^s, which may evolve with chemical reactions, Eq.(4.10.9)
relative fluid velocity	Element	Average element fluid velocity relative to mesh $\mathbf{w}$ in fluid and fluid-FSI materials
relative volume	Element	Relative volume $J = \det \mathbf{F}$
rigid acceleration	Rigid body	Rigid body center of mass acceleration
rigid angular acceleration	Rigid body	Rigid body angular acceleration
rigid angular momentum	Rigid body	Rigid body angular momentum
rigid angular position	Rigid body	Rigid body rotation pseudo-vector

rigid angular velocity	Rigid body	Rigid body angular velocity
rigid force	Rigid body	Total force applied to the rigid body
rigid kinetic energy	Rigid body	Rigid body kinetic energy
rigid linear momentum	Rigid body	Rigid body linear momentum
rigid position	Rigid body	Rigid body center of mass position
rigid rotation vector	Rigid body	Rigid body rotation pseudo-vector
rigid torque	Rigid body	Rigid body moment
rigid velocity	Rigid body	Rigid body center of mass velocity
sbm concentration	Element	Average element solid-bound molecule concentration
sbm referential apparent density	Element	Average element solid-bound molecule referential apparent density
shell director	Element	The shell director
shell relative volume	Element	Relative volume of shell element
shell strain	Element	Average strain in shell element
shell thickness	Node	Shell thickness
solute concentration	Element	Solute concentration c in biphasic-solute materials, or c^α in triphasic/multiphasic materials
solute flux	Element	Solute flux $\mathbf{j}$ in biphasic-solute materials, Eq.(4.8.4), or $\mathbf{j}^\alpha$ in triphasic/multiphasic materials, Eq.(4.9.9).
specific strain energy	Element	Average element specific strain energy
SPR principal stress	Element	Principal stress values obtained via SPR projection
SPR stress	Element	Cauchy stress obtained via SPR projection
SPR-P1 stress	Element	Cauchy stress obtained via SPR projection (first-order projection)
strain energy density	Element	Strain energy density $\Psi(\mathbf{C})$
stress	Element	Cauchy stress
surface traction	Surface	Nodal surface tractions of nodes on a contact surface
uncoupled pressure	Element	The pressure of an uncoupled material
ut4 nodal stress	Element	Stresses at the nodes of the UT4 element
vector gap	Element	The vector gap at nodes of a contact surface
velocity	Node	Nodal velocities (fluid nodal velocities in fluid analyses)
volume fraction	Element	Average element volume fraction of a solid mixture
in-situ target stretch	Element	the fiber stretch induced by the initial prestrain gradient
prestrain stretch	Element	the stretch induced by the effective prestrain gradient
prestrain correction	Element	the 3x3 prestrain correction tensor
SPR prestrain correction	Element	The 3x3 prestrain correction tensor (recovered with SPR)

The following example stores nodal displacements and element stresses.
Example:

```
<plotfile type="febio">
  <var type="displacement"/>
  <var type="stress"/>
</plotfile>
```

As of FEBio 2.4, additional information can be added in the type description of the variable definition. The general format is as follows.

```
<var type="name[filter]=alias"/>
```

The plot filter is defined by appending the name of the plot variable with the filter inside square brackets. Some plot variables require this to resolve possible ambiguities. For example,

```
<var type="solute concentration['solute1']"/>
```

This example will store the solute concentration of a solute named 'solute1' to the plot file.
The optional alias can be used to rename the variable. For example,

```
<var type="solute concentration['Na']=Na concentration"/>
```

This variable will store the solute concentration of a solute named 'Na' to the plot file using the name 'Na concentration'. This is the name that will be shown in PostView for instance.
Some variables require the specification of a named surface (* in above table). For example,

```
<var type="fluid surface force" surface="airfoil"/>
```

The named surface should be described in a *Surface* element (Section 3.6.5) within *Mesh* (Section 3.6).

Chapter 4

Materials

The following sections describe the material parameters for each of the available constitutive models, along with a short description of each material. A more detailed theoretical description of the constitutive models can be found in the *FEBio Theory Manual*.

4.1 Elastic Solids

This section describes the elastic materials, which are materials defined by a hyperelastic strain-energy function. A distinction will be made between so-called *compressible* and *uncoupled* materials. The former describe materials that can undergo volumetric compression. The latter are used for modeling (near-) incompressible materials.

4.1.1 Specifying Fiber Orientation or Material Axes

Some of the materials are transversely isotropic, requiring the specification of an initial material direction, which is called a *fiber* direction in FEBio. Other materials are orthotropic, requiring the specification of initial material axes that define the three planes of symmetry for those materials. Only one of these specifications should be provided. By default, material axes are aligned with the global Cartesian basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and the fiber direction is along $\mathbf{e}_1$. Local fiber or material axes orientation may be specified in several ways. FEBio gives the option to automatically generate the orientation, based on some user-specified parameters. However, the user can override this feature and specify the fiber or axes directions for each element manually in the *ElementData* section. See Section **??** for more details on how to do this.

4.1.1.1 Transversely Isotropic Materials

For transversely isotropic materials fiber orientation is specified with the *fiber* element. This element takes one attribute, namely *type*, which specifies the type of the fiber generator. The possible values are specified in the following table.

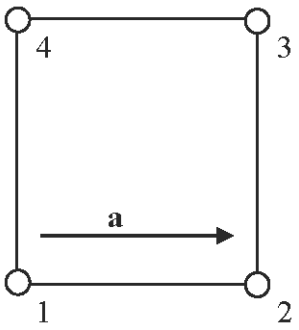
***type* Value**	**Description**
local	Use local element numbering (1)
vector	Define the fiber orientation as a constant vector (2)
spherical	specifies a spherical fiber distribution (3)
cylindrical	specifies a cylindrical fiber distribution (4)
angles	Specifies the fiber direction using spherical angles (5)

If the *type* attribute is omitted, the fiber distribution will follow the local element nodes 1 and 2. This would be the same as setting the fiber attribute to *local* and setting the value to "1,2".

Comments:

1. In this case, the fiber direction is determined by local element node numbering. The value is interpreted as the local node numbers of the nodes that define the direction of the fiber. The following example defines a local fiber axis by local element nodes 1 and 2. This option is very useful when the local fiber direction can be interpreted as following one of the mesh edges.

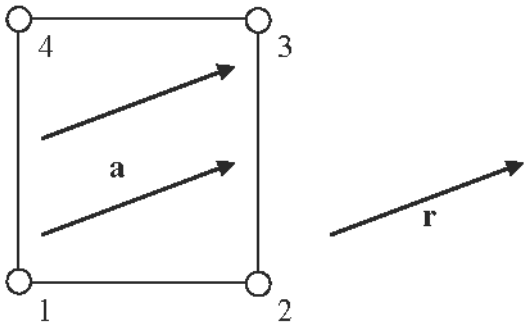
```
<fiber type="local">1,2</fiber>
```



***local* fiber direction option**

2. The fiber orientation is specified by a vector. The value is the direction of the fiber. The following defines all element fiber directions in the direction of the vector [1,0,0]:

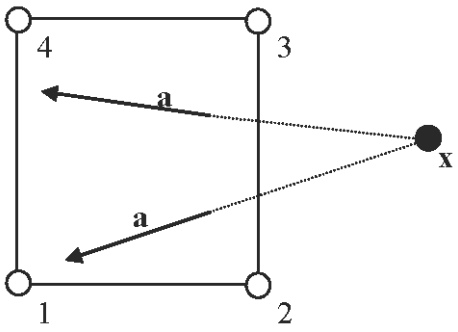
```
<fiber type="vector">1,0,0</fiber>
```



***vector* fiber direction option**

3. The fiber orientation is determined by a point in space and the global location of each element integration point. The value is the location of the point. The following example defines a spherical fiber distribution centered at [0,0,1]:

```
<fiber type="spherical">0,0,1</fiber>
```



***spherical* fiber direction option**

4. *cylindrical*: This type generates a fiber distribution that is cylindrical. The following subparameters must be defined.

   center defines the center of the cylinder

   axis defines the axis of the cylinder

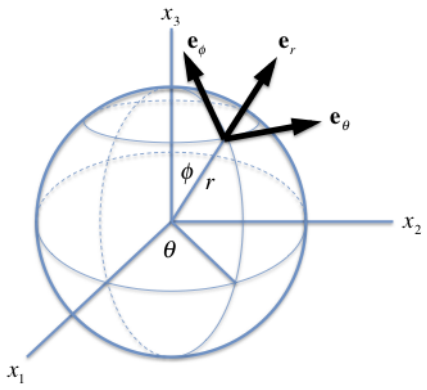
   vector defines a vector that will be transported around the cylinder

```
<fiber type="cylindrical">
  <center>0,0,0</center>
  <axis>0,0,1</axis>
  <vector>0,1,0</vector>
</fiber>
```

5. *angles*: This type generates a fiber orientation via the specification of spherical angles (azimuth and declination) relative to the local material axes (or global coordinate system, if no local material axes are defined). The following subparameters must be defined.

   theta azimuth angle (in degrees)

   phi declination angle (in degrees)



Spherical angles

The fiber is oriented along

$$\mathbf{e}_r = \cos\theta\sin\phi\,\mathbf{e}_1 + \sin\theta\sin\phi\,\mathbf{e}_2 + \cos\phi\,\mathbf{e}_3, 0 \leqslant \theta < 2\pi,\ 0 \leqslant \phi \leqslant \pi,$$

where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are orthonormal vectors representing the local element coordinate system (when specified, Section 4.1.1.2), or global coordinate system.

```
<fiber type="angles">
  <theta>20</center>
  <phi>90</phi>
</fiber>
```

When specifying a fiber direction $\mathbf{a}$, FEBio generates a set of orthogonal material axes as described in Section 4.1.1.2. generated with $\mathbf{d} = \boldsymbol{j}$, or else $\mathbf{d} = \boldsymbol{k}$ if $\mathbf{a}$ is collinear with $\boldsymbol{j}$ (where the triple $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$ refers to unit vectors defining the global coordinate system, i.e. $\boldsymbol{i} = (1, 0, 0)$, etc.). Because of the non-uniqueness of these material axes (only $\mathbf{e}_1$ is along a uniquely defined direction in a *fiber* element), caution should be used when material axes are compounded, as may occur in nested materials such as solid mixtures described in Sections 4.1.2.15 & 4.1.3.23. To enforce uniqueness, use the *mat_axis* element instead of the *fiber* element.

4.1.1.2 Orthotropic Materials

For orthotropic materials, the user needs to specify two fiber directions $\mathbf{a}$ and $\mathbf{d}$. From these FEBio will generate an orthonormal set of material axes vectors as follows:

$$\mathbf{e}_1 = \frac{\mathbf{a}}{\|\mathbf{a}\|}, \quad \mathbf{e}_2 = \mathbf{e}_3 \times \mathbf{e}_1, \quad \mathbf{e}_3 = \frac{\mathbf{a} \times \mathbf{d}}{\|\mathbf{a} \times \mathbf{d}\|}.$$

The vectors $\mathbf{a}$ and $\mathbf{d}$ are defined using the *mat_axis* element. This element takes a *type* attribute, which can take on the following values:

Value	Description
local	Use local element numbering (1)
vector	Specify the vectors $\mathbf{a}$ and $\mathbf{d}$ directly. (2)
angles	Specify the angles θ and φ [deg]. (3)

Comments:

1. When specifying *local* as the material axis type, the value is interpreted as a list of three local element node numbers. When specifying zero for all three, the default (1,2,4) is used.

```
<mat_axis type="local">0,0,0</mat_axis>
```

2. When using the *vector* type, you need to define the two generator vectors a and d. These are specified as child elements of the *mat_axis* element:

```
<mat_axis type="vector">
  <a>1,0,0</a>
  <d>0,1,0</d>
</mat_axis>
```

3. When using the *angle* type, you need to define the two angles θ and φ in degrees. These are specified as child elements of the *mat_axis* element:

```
<mat_axis type="angles">
  <theta>0</theta>
  <phi>90</phi>
</mat_axis>
```

The material axes $\{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\varphi\}$ are related to the global Cartesian basis (or local element axes) $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ via

$$\begin{aligned} \mathbf{e}_r &= \cos\theta \sin\phi\, \mathbf{e}_1 + \sin\theta \sin\phi\, \mathbf{e}_2 + \cos\phi\, \mathbf{e}_3 \\ \mathbf{e}_\theta &= -\sin\theta\, \mathbf{e}_1 + \cos\theta\, \mathbf{e}_2 \\ \mathbf{e}_\varphi &= -\cos\theta \cos\phi\, \mathbf{e}_1 - \sin\theta \cos\phi\, \mathbf{e}_2 + \sin\phi\, \mathbf{e}_3 \end{aligned} \quad .$$

4.1.2 Uncoupled Materials

Uncoupled, nearly-incompressible hyperelastic materials are described by a strain energy function that features an additive decomposition of the hyperelastic strain energy into deviatoric and dilational parts [51]:

$$\Psi\left(\mathbf{C}\right) = \tilde{\Psi}\left(\tilde{\mathbf{C}}\right) + U\left(J\right), \tag{4.1.1}$$

where $\tilde{\mathbf{C}} = \tilde{\mathbf{F}} \cdot \tilde{\mathbf{F}}^T$ and $\tilde{\mathbf{F}} = J^{-1/3}\mathbf{F}$ is the deviatoric part of the deformation gradient. The resulting 2^{nd} Piola-Kirchhoff stress is given by

$$\mathbf{S} = J^{-2/3}\,\mathrm{Dev}\left[\tilde{\mathbf{S}}\right] + pJ\mathbf{C}^{-1}, \tag{4.1.2}$$

where

$$\tilde{\mathbf{S}} = 2\frac{\partial\tilde{\Psi}}{\partial\tilde{\mathbf{C}}} \quad , \tag{4.1.3}$$

and

$$p := \frac{dU}{dJ}, \tag{4.1.4}$$

and $\mathrm{Dev}\left[\cdot\right]$ is the deviatoric operator in the material frame.

The corresponding Cauchy stress is given by

$$\boldsymbol{\sigma} = \mathrm{dev}\left[\tilde{\boldsymbol{\sigma}}\right] + p\mathbf{I}, \tag{4.1.5}$$

where $\tilde{\boldsymbol{\sigma}} = J^{-1}\tilde{\mathbf{F}} \cdot \tilde{\mathbf{S}} \cdot \tilde{\mathbf{F}}^T$ and $\mathrm{dev}\left[\cdot\right]$ is the deviatoric operator in the spatial frame.

For these materials, the entire bulk (volumetric) behavior is determined by the function $U\left(J\right)$, and p represents the entire hydrostatic stress. The function $U\left(J\right)$ is constructed to have a value of 0 for J =1 and to have a positive value for all other values of J >0.

All of these materials make use of the three-field element described by Simo and Taylor [51]. This element uses a trilinear interpolation of the displacement field and piecewise-constant interpolations for the pressure and volume ratio.

The uncoupled materials and the associated three-field element are very effective for representing nearly incompressible material behavior. Fully incompressible behavior can be obtained using an augmented Lagrangian method. To use the augmented Lagrangian method for enforcement of the incompressibility constraint to a user-defined tolerance, the user must define two additional material parameters:

Parameter	Description	Default
<laugon>	Turn augmented Lagrangian on for this material or off (1)	0 (off)
<atol>	Augmentation tolerance (2)	0.01

Comments:

1. A value of *1* (one) turns augmentation on, where a value of 0 (zero) turns it off.

2. The augmentation tolerance determines the convergence condition that is used for the augmented Lagrangian method: convergence is reached when the relative ratio of the lagrange multiplier norm of the previous augmentation $\|\lambda_k\|$ to the current one $\|\lambda_{k+1}\|$ is less than the specified value:

$$\left| \frac{\|\lambda_{k+1}\| - \|\lambda_k\|}{\|\lambda_{k+1}\|} \right| < \varepsilon.$$

Thus, a value of 0.01 implies that the change in norm between the previous augmentation loop and the current loop is less than 1%.

The augmented Lagrangian method for incompressibility enforcement is available for all materials that are based on an uncoupled hyperelastic strain energy function.

Example:

```
<material id="1" type="Mooney-Rivlin">
  <c1>5</c1>
  <c2>0.4</c2>
  <k>10000</k>
  <laugon>1</laugon> ← turns on augmented Lagrangian iterations
  <atol>0.05</atol> ← sets the augmentation tolerance
</material>
```

4.1.2.1 Arruda-Boyce

This material describes an incompressible Arruda-Boyce model [2]. The following material parameters are required:

<mu>	initial modulus	[**P**]
<N>	number of links in chain	[ ]
<k>	Bulk modulus	[**P**]

The uncoupled strain energy function for the Arruda-Boyce material is given by:

$$\Psi = \mu \sum_{i=1}^{5} \frac{C_i}{N^{i-1}} \left(\tilde{I}_1^i - 3^i \right) + U(J),$$

where, $C_1 = \frac{1}{2}, C_2 = \frac{1}{20}, C_3 = \frac{11}{1050}, C_4 = \frac{19}{7000}, C_5 = \frac{519}{673750}$ and $I_1$the first invariant of the right Cauchy-Green tensor. The volumetric strain function U is defined as follows,

$$U(J) = \frac{1}{2} k (\ln J)^2 .$$

This material model was proposed by Arruda and Boyce [2] and is based on an eight-chain representation of the macromolecular network structure of polymer chains. The strain energy form represents a truncated Taylor series of the inverse Langevin function, which arises in the statistical treatment of non-Gaussian chains. The parameter N is related to the locking stretch λ_L, the stretch at which the chains reach their full extended state, by $\lambda_L = \sqrt{N}$.

Example:

```
<material id="1" type="Arruda-Boyce">
  <mu>0.09</mu>
  <N>26.5</N>
  <k>100</k>
</material>
```

4.1.2.2 Ellipsoidal Fiber Distribution

The material type for an ellipsoidal continuous fiber distribution in an uncoupled formulation is "*EFD uncoupled*". Since fibers can only sustain tension, this material is not stable on its own. It must be combined with a stable compressible material that acts as a ground matrix, using a "*uncoupled solid mixture*" container as described in Section 4.1.2.15. The following material parameters need to be defined:

<beta>	parameters $(\beta_1, \beta_2, \beta_3)$	[ ]
<ksi>	parameters (ξ_1, ξ_2, ξ_3)	[**P**]

The stress $\tilde{\boldsymbol{\sigma}}$ for this material is given by [38, 3, 5]:

$$\tilde{\boldsymbol{\sigma}} = \int_0^{2\pi} \int_0^{\pi} H\left(\tilde{I}_n - 1\right) \tilde{\sigma}_n\left(\mathbf{n}\right) \sin\varphi \, d\varphi \, d\theta.$$

$\tilde{I}_n = \tilde{\lambda}_n^2 = \mathbf{N} \cdot \tilde{\mathbf{C}} \cdot \mathbf{N}$ is the square of the fiber stretch $\tilde{\lambda}_n$, $\mathbf{N}$ is the unit vector along the fiber direction (in the reference configuration), which in spherical angles is directed along (θ, φ), $\mathbf{n} = \tilde{\mathbf{F}} \cdot \mathbf{N} / \tilde{\lambda}_n$, and $H\left(.\right)$ is the unit step function that enforces the tension-only contribution. The fiber stress is determined from a fiber strain energy function in the usual manner,

$$\tilde{\sigma}_n = \frac{2\tilde{I}_n}{J} \frac{\partial \tilde{\Psi}}{\partial \tilde{I}_n} \mathbf{n} \otimes \mathbf{n} \, ,$$

where in this material,

$$\tilde{\Psi}\left(\mathbf{n}, \tilde{I}_n\right) = \xi\left(\mathbf{n}\right) \left(\tilde{I}_n - 1\right)^{\beta(\mathbf{n})} \, .$$

The materials parameters β and ξ are determined from:

$$\xi\left(\mathbf{n}\right) = \left(\frac{\cos^2\theta \sin^2\varphi}{\xi_1^2} + \frac{\sin^2\theta \sin^2\varphi}{\xi_2^2} + \frac{\cos^2\varphi}{\xi_3^2} \right)^{-1/2}$$
$$\beta\left(\mathbf{n}\right) = \left(\frac{\cos^2\theta \sin^2\varphi}{\beta_1^2} + \frac{\sin^2\theta \sin^2\varphi}{\beta_2^2} + \frac{\cos^2\varphi}{\beta_3^2} \right)^{-1/2} .$$

The orientation of the material axis can be defined as explained in detail in Section 4.1.1.

Example:

```
<material id="1" type="uncoupled solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>1</c1>
    <c2>0</c2>
    <k>1000</k>
  </solid>
  <solid type="EFD uncoupled">
    <ksi>10, 12, 15</ksi>
    <beta>2.5, 3, 3</beta>
    <k>15000</k>
  </solid>
</material>
```

4.1.2.3 Ellipsoidal Fiber Distribution Mooney-Rivlin

The material type for a Mooney-Rivlin material with an ellipsoidal continuous fiber distribution is "*EFD Mooney-Rivlin*". The following material parameters need to be defined:

<c1>	Mooney-Rivlin parameter c1	[**P**]
<c2>	Mooney-Rivlin parameter c2	[**P**]
<k>	bulk modulus	[**P**]
<beta>	parameters $(\beta_1, \beta_2, \beta_3)$	[ ]
<ksi>	parameters (ξ_1, ξ_2, ξ_3)	[**P**]

The stress $\tilde{\boldsymbol{\sigma}}$ for this material is given by,

$$\tilde{\boldsymbol{\sigma}} = \tilde{\boldsymbol{\sigma}}_{MR} + \tilde{\boldsymbol{\sigma}}_f \,.$$

Here, $\tilde{\boldsymbol{\sigma}}_{MR}$ is the stress from the Mooney-Rivlin basis (Section 4.1.2.8), and $\tilde{\boldsymbol{\sigma}}_f$ is the stress contribution from the ellipsoidal fiber distribution (Section 4.1.2.2). The orientation of the material axes can be defined as explained in detail in Section 4.1.1.

Example:

```
<material id="1" type="EFD Mooney-Rivlin">
  <c1>1</c1>
  <c2>0</c2>
  <beta>4.5,4.5,4.5</beta>
  <ksi>1,1,1</ksi>
  <k>20000</k>
  <mat_axis type="local">0,0,0</mat_axis>
</material>
```

4.1.2.4 Ellipsoidal Fiber Distribution Veronda-Westmann

The material type for a Veronda-Westmann material with an ellipsoidal continuous fiber distribution is "*EFD Veronda-Westmann*". The following material parameters need to be defined:

<c1>	First VW coefficient	[**P**]
<c2>	Second VW coefficient	[ ]
<k>	Bulk modulus	[**P**]
<beta>	parameters $(\beta_1, \beta_2, \beta_3)$	[ ]
<ksi>	parameters (ξ_1, ξ_2, ξ_3)	[**P**]

The stress $\tilde{\boldsymbol{\sigma}}$ for this material is given by,

$$\tilde{\boldsymbol{\sigma}} = \tilde{\boldsymbol{\sigma}}_{VW} + \tilde{\boldsymbol{\sigma}}_f \,.$$

Here, $\tilde{\boldsymbol{\sigma}}_{VW}$ is the stress from the Veronda-Westmann basis (Section 4.1.2.16), and $\tilde{\boldsymbol{\sigma}}_f$ is the stress contribution from the ellipsoidal fiber distribution (Section 4.1.2.2).

Example:

```
<material id="1" type="EFD Veronda-Westmann">
  <c1>1</c1>
  <c2>0.5</c2>
  <k>1000</k>
  <beta>4.5,4.5,4.5</beta>
  <ksi>1,1,1</ksi>
  <mat_axis type="local">0,0,0</mat_axis>
</material>
```

4.1.2.5 Fiber with Exponential-Power Law, Uncoupled Formulation

The material type for a single fiber with an exponential-power law, in an uncoupled strain energy formulation, is "*fiber-exp-pow-uncoupled*". Since fibers can only sustain tension, this material is not stable on its own. It must be combined with a stable uncoupled material that acts as a ground matrix, using a "*uncoupled solid mixture*" container as described in Section 4.1.2.15. The following material parameters need to be defined:

<ksi>	ξ, representing a measure of the fiber modulus	[**P**]
<alpha>	α, coefficient of exponential argument	[ ]
<beta>	β, power of exponential argument	[ ]

The fiber is oriented along the unit vector $\mathbf{e}_1$, where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are orthonormal basis vectors representing the local element coordinate system when specified (Section 4.1.1), or else the global Cartesian coordinate system. The stress $\tilde{\boldsymbol{\sigma}}$ for this fibrous material is given by

$$\tilde{\boldsymbol{\sigma}} = H\left(\tilde{I}_n - 1\right)\frac{2\tilde{I}_n}{J}\frac{\partial\tilde{\Psi}}{\partial\tilde{I}_n}\mathbf{n}\otimes\mathbf{n},$$

where $\tilde{I}_n = \tilde{\lambda}_n^2 = \mathbf{N}\cdot\tilde{\mathbf{C}}\cdot\mathbf{N}$ is the square of the fiber stretch, $\mathbf{n} = \tilde{\mathbf{F}}\cdot\mathbf{N}/\tilde{\lambda}_n$, and $H(.)$ is the unit step function that enforces the tension-only contribution.. The fiber strain energy density is given by

$$\tilde{\Psi} = \frac{\xi}{\alpha\beta}\left(\exp\left[\alpha\left(\tilde{I}_n - 1\right)^{\beta}\right] - 1\right),$$

where $\xi > 0$, $\alpha \geqslant 0$, and $\beta \geqslant 2$.

Note: In the limit when $\alpha \to 0$, this expressions produces a power law,

$$\lim_{\alpha\to 0}\tilde{\Psi} = \frac{\xi}{\beta}\left(\tilde{I}_n - 1\right)^{\beta}.$$

Note: When $\beta > 2$, the fiber modulus is zero at the strain origin ($\tilde{I}_n = 1$). Therefore, use $\beta > 2$ when a smooth transition in the stress is desired from compression to tension.

Example:

Single fiber oriented along $\mathbf{e}_1$, embedded in a neo-Hookean ground matrix.

```
<material id="1" type="uncoupled solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>10.0</c1>
    <c2>0</c2>
    <k>10e3</k>
  </solid>
  <solid type="fiber-exp-pow-uncoupled">
    <ksi>5</ksi>
    <alpha>20</alpha>
    <beta>3</beta>
    <k>5e3</k>
    <mat_axis type="angles">
        <theta>0</theta>
```

```
        <phi>90</phi>
    </mat_axis>
  </solid>
</material>
```

Example:

Two fibers in the plane orthogonal to $\mathbf{e}_1$, oriented at ±25 degrees relative to $\mathbf{e}_3$, embedded in a Mooney-Rivlin ground matrix.

```
<material id="1" type="uncoupled solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>10.0</c1>
    <c2>0</c2>
    <k>10e3</k>
  </solid>
  <solid type="fiber-exp-pow">
    <ksi>5</ksi>
    <alpha>20</alpha>
    <beta>3</beta>
    <k>5e3</k>
    <mat_axis type="angles">
        <theta>90</theta>
        <phi>25</phi>
    </mat_axis>
  </solid>
  <solid type="fiber-exp-pow">
    <ksi>5</ksi>
    <alpha>20</alpha>
    <beta>3</beta>
    <k>5e3</k>
    <mat_axis type="angles">
        <theta>-90</theta>
        <phi>25</phi>
    </mat_axis>
  </solid>
</material>
```

4.1.2.6 Fiber with Toe-Linear Response, Uncoupled Formulation

This material type is "*fiber-pow-linear-uncoupled*". The following material parameters need to be defined:

<E>	E, the fiber modulus in the linear range ($E \geqslant 0$)	[**P**]
<beta>	β, the power-law exponent in the toe region ($\beta \geqslant 2$)	[ ]
<lam0>	λ_0, the stretch ratio when the toe region transitions to the linear region ($\lambda_0 > 1$)	[ ]

The fiber strain energy density is given by

$$\tilde{\Psi}_n\left(\tilde{I}_n\right) = \begin{cases} 0 & \tilde{I}_n < 1 \\ \frac{\xi}{2\beta}\left(\tilde{I}_n - 1\right)^{\beta} & 1 \leqslant \tilde{I}_n \leqslant I_0 \\ E\left(I_0^{1/2} - \tilde{I}_n^{1/2}\right) + B\left(\tilde{I}_n - I_0\right) + \Psi_0 & I_0 < \tilde{I}_n \end{cases},$$

where $I_0 = \lambda_0^2$,

$$\xi = \frac{E}{2\left(\beta - 1\right)}\left(I_0 - 1\right)^{2-\beta},\ B = \frac{E}{2}\left[\frac{\left(I_0 - 1\right)}{2\left(\beta - 1\right)} + I_0\right],\ \Psi_0 = \frac{\xi}{2\beta}\left(I_0 - 1\right)^{\beta}$$

Example:

```
<material type="fiber-power-linear-uncoupled">
  <fiber type="angles">
    <theta>20</center>
    <phi>90</phi>
  </fiber>
  <E>1</E>
  <beta>2.5</beta>
  <lam0>1.06</lam0>
</material>
```

4.1.2.7 Fung Orthotropic

The material type for orthotropic Fung elasticity [27, 26] is "*Fung orthotropic*". The following material parameters must be defined:

<E1>	E_1 Young's modulus	**[P]**
<E2>	E_2 Young's modulus	**[P]**
<E3>	E_3 Young's modulus	**[P]**
<G12>	G_{12} shear modulus	**[P]**
<G23>	G_{23} shear modulus	**[P]**
<G31>	G_{31} shear modulus	**[P]**
<v12>	ν_{12} Poisson's ratio	[ ]
<v23>	ν_{23} Poisson's ratio	[ ]
<v31>	ν_{31} Poisson's ratio	[ ]
<c>	c coefficient	**[P]**
<k>	bulk modulus	**[P]**

The hyperelastic strain energy function is given by [4],

$$\Psi = \frac{1}{2}c\left(e^{\tilde{Q}} - 1\right) + U\left(J\right) , \tag{4.1.6}$$

where,

$$\tilde{Q} = c^{-1}\sum_{a=1}^{3}\left[2\mu_a\mathbf{M}_a : \tilde{\mathbf{E}}^2 + \sum_{b=1}^{3}\lambda_{ab}\left(\mathbf{M}_a : \tilde{\mathbf{E}}\right)\left(\mathbf{M}_b : \tilde{\mathbf{E}}\right)\right] .$$

Here, $\tilde{\mathbf{E}} = \left(\tilde{\mathbf{C}} - \mathbf{I}\right)/2$ and $\mathbf{M}_a = \mathbf{V}_a \otimes \mathbf{V}_a$ where $\mathbf{V}_a$ defines the initial direction of material axis a. See Section 4.1.1.2 on how to define the material axes for orthotropic materials. The Lamé constants μ_a $(a = 1, 2, 3)$ and λ_{ab} $(a, b = 1, 2, 3,\ \lambda_{ba} = \lambda_{ab})$ are related to Young's moduli E_a, shear moduli G_{ab} and Poisson's ratios ν_{ab} via

$$\begin{bmatrix} \lambda_{11}+2\mu_1 & \lambda_{12} & \lambda_{13} & 0 & 0 & 0 \\ \lambda_{12} & \lambda_{22}+2\mu_2 & \lambda_{23} & 0 & 0 & 0 \\ \lambda_{13} & \lambda_{23} & \lambda_{33}+2\mu_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}\left(\mu_1+\mu_2\right) & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}\left(\mu_2+\mu_3\right) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}\left(\mu_1+\mu_3\right) \end{bmatrix}^{-1}$$

$$= \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{12}}{E_1} & -\frac{\nu_{13}}{E_1} & 0 & 0 & 0 \\ -\frac{\nu_{21}}{E_2} & \frac{1}{E_2} & -\frac{\nu_{23}}{E_2} & 0 & 0 & 0 \\ -\frac{\nu_{31}}{E_3} & -\frac{\nu_{32}}{E_3} & \frac{1}{E_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{12}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{23}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{31}} \end{bmatrix} .$$

The orthotropic Lamé parameters should produce a positive definite stiffness matrix.

Example:

```
<material id="3" type="Fung orthotropic">
```

```
    <E1>124</E1>
    <E2>124</E2>
    <E3>36</E3>
    <G12>67</G12>
    <G23>40</G23>
    <G31>40</G31>
    <v12>-0.075</v12>
    <v23>0.87</v23>
    <v31>0.26</v31>
    <c>1</c>
    <k>120000</k>
  </material>
```

4.1.2.8 Mooney-Rivlin

The material type for uncoupled Mooney-Rivlin materials is *Mooney-Rivlin*. The following material parameters must be defined:

<c1>	Coefficient of first invariant term	[**P**]
<c2>	Coefficient of second invariant term	[**P**]
<k>	Bulk modulus	[**P**]

This material model is a hyperelastic Mooney-Rivlin type with uncoupled deviatoric and volumetric behavior. The strain-energy function is given by:

$$\Psi = C_1 \left(\tilde{I}_1 - 3 \right) + C_2 \left(\tilde{I}_2 - 3 \right) + \frac{1}{2} K \left(\ln J \right)^2 .$$

C_1 and C_2 are the Mooney-Rivlin material coefficients. The variables $\tilde{I}_1$ and $\tilde{I}_2$ are the first and second invariants of the deviatoric right Cauchy-Green deformation tensor $\tilde{\mathbf{C}}$. The coefficient K is a bulk modulus-like penalty parameter and J is the determinant of the deformation gradient tensor. When $C_2 = 0$, this model reduces to an uncoupled version of the neo-Hookean constitutive model.

This material model uses a three-field element formulation, interpolating displacements as linear field variables and pressure and volume ratio as piecewise constant on each element [51].

This material model is useful for modeling certain types of isotropic materials that exhibit some limited compressibility, i.e. 100 < (K/C_1) < 10000.

Example:

```
<material id="2" type="Mooney-Rivlin">
  <c1>10.0</c1>
  <c2>20.0</c2>
  <k>1000</k>
</material>
```

4.1.2.9 Muscle Material

This material model implements the constitutive model developed by Silvia S. Blemker [18]. The material type for the muscle material is *muscle material*. The model is designed to simulate the passive and active material behavior of skeletal muscle. It defines the following parameters:

<g1>	along fiber shear modulus	[**P**]
<g2>	cross fiber shear modulus	[**P**]
<p1>	exponential stress coefficients	[**P**]
<p2>	fiber uncrimping factor	[ ]
<Lofl>	optimal fiber length	[ ]
<smax>	maximum isometric stress	[**P**]
<lambda>	fiber stretch for straightened fibers	[ ]
<k>	bulk modulus	[**P**]
<active_contraction>	activation level	

The main difference between this material formulation compared to other transversely hyperelastic materials is that it is formulated using a set of new invariants, originally due to Criscione [23], instead of the usual five invariants proposed by A.J.M. Spencer [53]. For this particular material, only two of the five Criscione invariants are used. The strain energy function is defined as follows:

$$\Psi\left(B_1, B_2, \lambda\right) = G_1\tilde{B}_1^2 + G_2\tilde{B}_2^2 + F_m\left(\tilde{\lambda}\right) + U\left(J\right).$$

The function $F_m$is the strain energy contribution of the muscle fibers. It is defined as follows:

$$\lambda\frac{\partial F_m}{\partial\lambda} = \sigma_{\max}\left(f_m^{\text{passive}}\left(\lambda\right) + \alpha f_m^{\text{active}}\left(\lambda\right)\right)\frac{\lambda}{\lambda_{ofl}},$$

where,

$$f_m^{\text{passive}}\left(\lambda\right) = \begin{cases} 0 & \lambda \leqslant \lambda_{ofl} \\ P_1\left(e^{P_2\left(\lambda/\lambda_{ofl}-1\right)} - 1\right) & \lambda_{ofl} < \lambda < \lambda^* \\ P_3\lambda/\lambda_{ofl} + P_4 & \lambda \geqslant \lambda^* \end{cases},$$

and

$$f_m^{\text{active}}\left(\lambda\right) = \begin{cases} 9\left(\lambda/\lambda_{ofl} - 0.4\right)^2 & \lambda \leqslant 0.6\lambda_{ofl} \\ 9\left(\lambda/\lambda_{ofl} - 1.6\right)^2 & \lambda \geqslant 1.4\lambda_{ofl} \\ 1 - 4\left(1 - \lambda/\lambda_{ofl}\right)^2 & 0.6\lambda_{ofl} < \lambda < 1.4\lambda_{ofl} \end{cases}.$$

The values $P_3$and P_4 are determined by requiring $C^0$and C^1continuity at $\lambda = \lambda^*$.

The parameter α is the activation level and can be specified using the *active_contraction* element. You can specify a loadcurve using the *lc* attribute. The value is interpreted as a scale factor when a loadcurve is defined or as the constant activation level when no loadcurve is defined.

The muscle fiber direction is specified similarly to the transversely isotropic Mooney-Rivlin model.

Example:

```
<material id="1" type="muscle material">
  <g1>500</g1>
  <g2>500</g2>
```

```
    <p1>0.05</p1>
    <p2>6.6</p2>
    <smax>3e5</smax>
    <Lofl>1.07</Lofl>
    <lambda>1.4</lambda>
    <k>1e6</k>
    <fiber type="vector">1,0,0</fiber>
  </material>
```

4.1.2.10 Ogden

This material describes an incompressible hyperelastic Ogden material [51]. The following material parameters must be defined:

<c[n]>	Coefficient of n^{th} term, where n can range from 1 to 6	[**P**]
<m[n]>	Exponent of n^{th} term, where n can range from 1 to 6	[ ]
<k>	Bulk modulus	[**P**]

The uncoupled hyperelastic strain energy function for this material is given in terms of the eigenvalues of the deformation tensor:

$$\Psi = \sum_{i=1}^{N} \frac{c_i}{m_i^2} \left(\tilde{\lambda}_1^{m_i} + \tilde{\lambda}_2^{m_i} + \tilde{\lambda}_3^{m_i} - 3 \right) + U\left(J\right).$$

Here, $\tilde{\lambda}_i^2$ are the eigenvalues of $\tilde{\mathbf{C}}$, $c_i$and $m_i$are material coefficients and N ranges from 1 to 6. Note that you only have to include the material parameters for the terms you intend to use.

Example:

```
<material id="1" type="Ogden">
  <m1>2.4</m1>
  <c1>1</c1>
  <k>100</k>
</material>
```

4.1.2.11 Tendon Material

The material type for the tendon material is *tendon material*. The tendon material is similar to the muscle material [18]. The only difference is the fiber function. For tendon material this is defined as:

$$\lambda \frac{\partial F_t}{\partial \lambda} = \sigma(\lambda),$$

where

$$\sigma(\lambda) = \begin{cases} 0 & \lambda \leqslant 1 \\ L_1\left(e^{L_2(\lambda-1)} - 1\right) & 1 < \lambda < \lambda^* \\ L_3\lambda + L_4 & \lambda \geqslant \lambda^* \end{cases}.$$

The parameters $L_3$and $L_4$are determined by requiring C^0 and C^1 continuity at λ^*.

The material parameters for this material are listed below.

<g1>	along fiber shear modulus	[**P**]
<g2>	cross fiber shear modulus	[**P**]
<l1>	exponential stress coefficients	[**P**]
<l2>	fiber uncrimping factor	[ ]
<lambda>	fiber stretch for straightened fibers	[ ]
<k>	bulk modulus	[**P**]

The tendon fiber direction is specified similarly to the transversely isotropic Mooney-Rivlin model.

Example:

```
<material id="1" type="tendon material">
  <g1>5e4</g1>
  <g2>5e4</g2>
  <l1>2.7e6/l1>
  <l2>46.4</l2>
  <lambda>1.03</lambda>
  <k>1e7</k>
  <fiber type="vector">1,0,0</fiber>
</material>
```

4.1.2.12 Tension-Compression Nonlinear Orthotropic

The material type for the tension-compression nonlinear orthotropic material is "*TC nonlinear orthotropic*". The following material parameters are defined:

<c1>	First Mooney-Rivlin material parameter	[**P**]
<c2>	Second Mooney-Rivlin material parameter	[**P**]
<k>	bulk modulus	[**P**]
<beta>	the β parameter (see below)	[ ]
<ksi>	the ξ parameter (see below)	[**P**]
<mat_axis>	defines the material axes	

This material is based on the following uncoupled hyperelastic strain energy function [11]:

$$\Psi\left(\mathbf{C},\lambda_1,\lambda_2,\lambda_3\right)=\tilde{\Psi}_{iso}\left(\tilde{\mathbf{C}}\right)+\sum_{i=1}^{3}\tilde{\Psi}_i^{TC}\left(\tilde{\lambda}_i\right)+U\left(J\right)\ .$$

The isotropic strain energy $\tilde{\Psi}_{iso}$and the dilatational energy U are the same as for the Mooney-Rivlin material. The tension-compression term is defined as follows:

$$\tilde{\Psi}_i^{TC}\left(\tilde{\lambda}_i\right)=\begin{cases}\xi_i\left(\tilde{\lambda}_i-1\right)^{\beta_i} & \tilde{\lambda}_i>1\\ 0 & \tilde{\lambda}_i\leqslant 1\end{cases}\qquad \xi_i\geqslant 0\quad \text{(no sum over } i\text{)}\ .$$

The $\tilde{\lambda}_i$ parameters are the deviatoric fiber stretches of the local material fibers:

$$\tilde{\lambda}_i=\left(\mathbf{a}_i^0\cdot\tilde{\mathbf{C}}\cdot\mathbf{a}_i^0\right)^{1/2}\ .$$

The local material fibers are defined (in the reference frame) as an orthonormal set of vectors $\mathbf{a}_i^0$. See Section 4.1.1 for more information. As with all uncoupled materials, this material uses the three-field element formulation.

A complete example for this material follows.

```
<material id="7" name="cartilage" type="TC nonlinear orthotropic">
  <c1>1.0</c1>
  <c2>0.0</c2>
  <k>100</k>
  <beta>4.3,4.3,4.3</beta>
  <ksi>4525, 4525, 4525</ksi>
  <mat_axis type="local">0,0,0</mat_axis>
</material>
```

4.1.2.13 Transversely Isotropic Mooney-Rivlin

The material type for transversely isotropic Mooney-Rivlin materials is "*trans iso Mooney-Rivlin*". The following material parameters must be defined:

<c1>	Mooney-Rivlin coefficient 1	[**P**]
<c2>	Mooney-Rivlin coefficient 2	[**P**]
<c3>	Exponential stress coefficient	[**P**]
<c4>	Fiber uncrimping coefficient	[ ]
<c5>	Modulus of straightened fibers	[**P**]
<k>	Bulk modulus	[**P**]
<lam_max>	Fiber stretch for straightened fibers	[ ]
<fiber>	Fiber distribution option	

This constitutive model can be used to represent a material that has a single preferred fiber direction and was developed for application to biological soft tissues [47, 48, 59]. It can be used to model tissues such as tendons, ligaments and muscle. The elastic response of the tissue is assumed to arise from the resistance of the fiber family and an isotropic matrix. It is assumed that the uncoupled strain energy function can be written as follows:

$$\Psi = F_1\left(\tilde{I}_1, \tilde{I}_2\right) + F_2\left(\tilde{\lambda}\right) + \frac{K}{2}\left[\ln\left(J\right)\right]^2.$$

Here $\tilde{I}_1$ and $\tilde{I}_2$ are the first and second invariants of the deviatoric version of the right Cauchy Green deformation tensor $\tilde{\mathbf{C}}$ and $\tilde{\lambda}$ is the deviatoric part of the stretch along the fiber direction ($\tilde{\lambda}^2 = \mathbf{a}_0 \cdot \tilde{\mathbf{C}} \cdot \mathbf{a}_0$, where $\mathbf{a}_0$ is the initial fiber direction), and $J = \det\left(\mathbf{F}\right)$ is the Jacobian of the deformation (volume ratio). The function F_1 represents the material response of the isotropic ground substance matrix and is the same as the Mooney-Rivlin form specified above, while F_2 represents the contribution from the fiber family. The strain energy of the fiber family is as follows:

$$F_2\left(\tilde{\lambda}\right) = \begin{cases} 0 & \tilde{\lambda} \leqslant 1 \\ C_3\left(e^{-C_4}\left(\mathrm{Ei}\left(C_4\tilde{\lambda}\right) - \mathrm{Ei}\left(C_4\right)\right) - \ln\tilde{\lambda}\right) & 1 < \tilde{\lambda} < \lambda_m \\ C_5\left(\tilde{\lambda} - 1\right) + C_6 \ln\tilde{\lambda} & \tilde{\lambda} \geqslant \lambda_m \end{cases}$$

where $\mathrm{Ei}\left(\cdot\right)$ is the exponential integral function. The resulting fiber stress is evaluated from

$$\tilde{\lambda}\frac{\partial F_2}{\partial \tilde{\lambda}} = \begin{cases} 0 & \tilde{\lambda} \leqslant 1 \\ C_3\left(e^{C_4\left(\tilde{\lambda}-1\right)} - 1\right) & 1 < \tilde{\lambda} < \lambda_m \\ C_5\tilde{\lambda} + C_6 & \tilde{\lambda} \geqslant \lambda_m \end{cases}.$$

Here, C_1 and C_2 are the Mooney-Rivlin material coefficients, *lam_max* (λ_m) is the stretch at which the fibers are straightened, C_3scales the exponential stresses, C_4 is the rate of uncrimping of the fibers, and $C_5$is the modulus of the straightened fibers. C_6 is determined from the requirement that the stress is continuous at λ_m.

This material model uses a three-field element formulation, interpolating displacements as linear field variables and pressure and volume ratio as piecewise constant on each element [51].

The fiber orientation can be specified as explained in Section 4.1.1. Active stress along the fiber direction can be simulated using an active contraction model. To use this feature you need to define the *active_contraction* material. This material has a *ascl* property that takes an optional attribute, *lc*, which defines the loadcurve. There are also several options:

<ascl>	Activation scale factor (default=0)
<ca0>	Intracellular calcium concentration (default=1)
<camax>	Maximum peak intracellular calcium concentration (default=ca0)
<beta>	tension-sarcomere length relation constant
<l0>	No tension sarcomere length
<refl>	Unloaded sarcomere length
<Tmax>	Isometric tension under maximal activation at camax (default=1)

Example:

This example defines a transversely isotropic material with a Mooney-Rivlin basis. It defines a homogeneous fiber direction and uses the active fiber contraction feature.

```
<material id="3" type="trans iso Mooney-Rivlin">
  <c1>13.85</c1>
  <c2>0.0</c2>
  <c3>2.07</c3>
  <c4>61.44</c4>
  <c5>640.7</c5>
  <k>100.0</k>
  <lam_max>1.03</lam_max>
  <fiber type="vector">1,0,0</fiber>
  <active_contraction>
    <ascl lc="1">1</ascl>
    <ca0>4.35</ca0>
    <beta>4.75</beta>
    <l0>1.58</l0>
    <refl>2.04</refl>
  </active_contraction>
</material>
```

4.1.2.14 Transversely Isotropic Veronda-Westmann

The material type for transversely isotropic Veronda-Westmann materials is "*trans iso Veronda-Westmann*" [58]. The following material parameters must be defined:

<c1>	Veronda-Westmann coefficient 1	[**P**]
<c2>	Veronda-Westmann coefficient 2	[ ]
<c3>	Exponential stress coefficient	[**P**]
<c4>	Fiber uncrimping coefficient	[ ]
<c5>	Modulus of straightened fibers	[**P**]
<k>	Bulk modulus	[**P**]
<lam_max>	Fiber stretch for straightened fibers	[ ]
<fiber>	Fiber distribution option.	

This uncoupled hyperelastic material differs from the Transversely Isotropic Mooney-Rivlin model in that it uses the Veronda-Westmann model for the isotropic matrix. The interpretation of the material parameters, except C_1 and $C_2$is identical to this material model.

The fiber distribution option is explained in Section 4.1.1. An active contraction model can also be defined for this material. See the transversely isotropic Mooney-Rivlin model for more details (Section 4.1.2.13).

Example:

This example defines a transversely isotropic material model with a Veronda-Westmann basis. The fiber direction is implicitly implied as *local*.

```
<material id="3" type="trans iso Veronda-Westmann">
  <c1>13.85</c1>
  <c2>0.0</c2>
  <c3>2.07</c3>
  <c4>61.44</c4>
  <c5>640.7</c5>
  <lam_max>1.03</lam_max>
</material>
```

4.1.2.15 Uncoupled Solid Mixture

This material describes a mixture of quasi-incompressible elastic solids. It is a container for any combination of the materials described in Section 4.1.2.

<solid>	Container tag for compressible material	

The mixture may consist of any number of solids. The stress tensor for the solid mixture is the sum of the stresses for all the solids. The bulk modulus of the uncoupled solid mixture is the sum of the bulk moduli of the individual <solid> materials. A bulk modulus specified outside of the <solid> materials will be ignored.

Material axes may be optionally specified within the <material> level, as well as within each <solid>. Within the <material> level, these represent the local element axes relative to the global coordinate system. Within the <solid>, they represent local material axes relative to the element. If material axes are specified at both levels, they are properly compounded to produce local material axes relative to the global coordinate system. Material axes specified in the <ElementData> section are equivalent to a specification at the <material> level: they correspond to local element axes relative to the global system.

Example:

```
<material id="1" type="uncoupled solid mixture">
  <mat_axis type="vector">
    <a>1,0,0</a>
    <d>0,1,0</d>
  </mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>2.0</c1>
    <c2>0.0</c2>
    <k>2000</k>
  </solid>
  <solid type="EFD uncoupled">
    <mat_axis type="vector">
      <a>0.8660254,0.5,0</a>
      <d>0,0,1</d>
    </mat_axis>
    <ksi>5, 1, 1</ksi>
    <beta>2.5, 3, 3</beta>
    <k>15e3</k>
  </solid>
  <solid type="EFD uncoupled">
    <mat_axis type="vector">
      <a>0.8660254,-0.5,0</a>
      <d>0,0,1</d>
    </mat_axis>
    <ksi>5, 1, 1</ksi>
    <beta>2.5, 3, 3</beta>
    <k>15e3</k>
  </solid>
</material>
```

4.1.2.16 Veronda-Westmann

The material type for incompressible Veronda-Westmann materials is *Veronda-Westmann* [55]. The following material parameters must be defined:

<c1>	First VW coefficient	[**P**]
<c2>	Second VW coefficient	[ ]
<k>	Bulk modulus	[**P**]

This model is similar to the Mooney-Rivlin model in that it also uses an uncoupled deviatoric dilatational strain energy:

$$\Psi = C_1 \left[e^{\left(C_2\left(\tilde{I}_1 - 3\right)\right)} - 1 \right] - \frac{C_1 C_2}{2} \left(\tilde{I}_2 - 3 \right) + U\left(J\right) .$$

The dilatational term is identical to the one used in the Mooney-Rivlin model. This model can be used to describe certain types of biological materials that display exponential stiffening with increasing strain. It has been used to describe the response of skin tissue [55].

Example:

```
<material id="2" type="Veronda-Westmann">
  <c1>1000.0</c1>
  <c2>2000.0</c2>
  <k>1000</k>
</material>
```

4.1.2.17 Mooney-Rivlin Von Mises Distributed Fibers

(Sclera and other thin soft tissues)

Authors: Cécile L.M. Gouget and Michaël J.A. Girard

The material type for a thin material where fiber orientation follows a von Mises distribution is "Mooney-Rivlin von Mises Fibers". The following parameters must be defined:

<c1>	Mooney-Rivlin coefficient 1	[**P**]
<c2>	Mooney-Rivlin coefficient 2	[**P**]
<c3>	Exponential stress coefficient	[**P**]
<c4>	Fiber uncrimping coefficient	[ ]
<c5>	Modulus of straightened fibers	[**P**]
<k>	Bulk modulus	[**P**]
<lam_max>	Fiber stretch for straightened fibers	[ ]
<tp>	Preferred fiber orientation in radian (angle within the plane of the fibers, defined with respect to the first direction given in mat_axis)	[rad]
<kf>	Fiber concentration factor	[ ]
<vmc>	Choice of von Mises distribution	
	=1 semi-circular von Mises distribution	
	=2 constrained von Mises mixture distribution	
<var_n>	Exponent (only for vmc=2)	
<gipt>	Number of integration points (value is a multiple of 10)	
<mat_axis>	Reference frame of the plane of the fibers	

This constitutive model is designed for thin soft tissues. Fibers are multi-directional: they are distributed within the plane tangent to the tissue surface and they follow a unimodal distribution. It is a constitutive model that is suitable for ocular tissues (e.g. sclera and cornea) but can be used for other thin soft tissues. The proposed strain energy function is as follows:

$$\Psi = F_1\left(\tilde{I}_1, \tilde{I}_2\right) + \int_{\theta_P-\pi/2}^{\theta_P+\pi/2} P\left(\theta\right) F_2\left(\tilde{\lambda}\left[\theta\right]\right) d\theta + \frac{K}{2}\left[\ln\left(J\right)\right]^2,$$

where P is the 2D unimodal distribution function of the fibers which satisfies the normalization condition:

$$\int_{\theta_P-\pi/2}^{\theta_P+\pi/2} P\left(\theta\right) d\theta = 1.$$

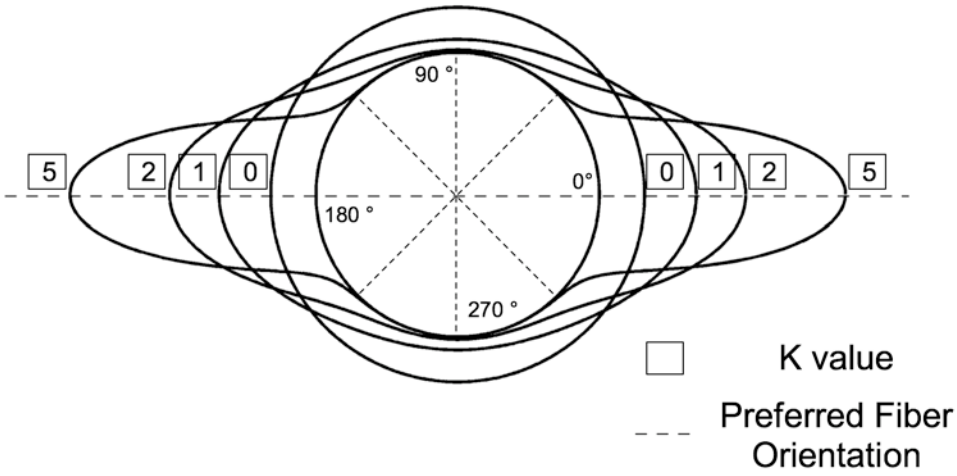
θ_P is the preferred fiber orientation relative to a local coordinate system (parameter tp). The functions $F_1$and F_2 are described in the "Transversely Isotropic Mooney-Rivlin" model. The user can choose between 2 distribution functions using the parameter vmc.

1. Semi-circular von Mises distribution (vmc = 1) [30]

The semi-circular von Mises distribution is one of the simplest unimodal distribution in circular statistics. It can be expressed as

$$P(\theta) = \frac{1}{\pi I_0(k_f)} \exp\left[k_f \cos\left(2(\theta - \theta_p)\right)\right],$$

where I_0 is the modified Bessel function of the first kind (order 0), and k_f is the fiber concentration factor. k_f controls the amount of fibers that are concentrated along the orientation θ_P as illustrated in the figure below.



Polar representation of the semi-circular von-Mises distribution describing in-plane collagen fiber alignment. In this case, the preferred fiber orientation θ_P is equal to zero degrees. When the fiber concentration factor k is equal to zero, the collagen fibers have an isotropic distribution in a plane tangent to the scleral wall. As k increases, the collagen fibers align along the preferred fiber orientation θ_P. Note that the distributions were plotted on a circle of unit one to ease visualization.

2. Constrained von Mises Mixture Distribution (vmc = 2) [31]

The semi-circular von Mises distribution is ideal for its simplicity but in some instance it fails to accurately describe the isotropic subpopulation of fibers present in thin soft tissues. An improved mathematical description is proposed here as a weighted mixture of the semi-circular uniform distribution and the semi-circular von Mises distribution. It can be expressed as:

$$P(\theta) = \frac{1-\beta}{\pi} + \frac{\beta}{\pi I_0(k_f)} \exp\left[k_f \cos\left(2(\theta - \theta_p)\right)\right],$$

where β needs to be constrained for uniqueness and stability. β is expressed as:

$$\beta = \left(\frac{I_1(k_f)}{I_0(k_f)}\right)^n,$$

where I_1 is the modified Bessel function of the first kind (order 1), and n is an exponent to be determined experimentally (parameter var_n). n=2 has been found to be suitable for the sclera based on fiber distribution measurements using small angle light scattering.

Note about Numerical Integration

All numerical integrations are performed using a 10-point Gaussian quadrature rule. The number of Gaussian integration points can be increased for numerical stability. This is controlled through the parameter *gipt*. We recommend to use at least *gipt* = 20 (2×10 integration points).

Note that the more integration points are used, the slower the model will run. By increasing the number of integration points, one should observe convergence in the numerical accuracy. The parameter gipt is required to be a multiple of 10.

Definition of the Fiber Plane

The user must specify two directions to define a local coordinate system of the plane in which the fibers lay. As explained in Section 4.1.1.2, this can be done by defining two directions with the parameter *mat_axis*. The first direction (vector $\mathbf{a}$ of *mat_axis*) must be the reference direction used to define the angle *tp* (θ_P). The second direction (vector $\mathbf{d}$ of mat_axis) can be any other direction in the plane of the fibers. Thus, a fiber at angle θ_P will be along the vector $\mathbf{v} = \cos\theta_P \mathbf{e}_1 + \sin\theta_P \mathbf{e}_2$ where $\mathbf{e}_1 = \mathbf{a}/\left\|\mathbf{a}\right\|$, $\mathbf{e}_2 = \left(\mathbf{e}_3 \times \mathbf{a}\right)/\left\|\mathbf{e}_3 \times \mathbf{a}\right\|$, $\mathbf{e}_3 = \left(\mathbf{a} \times \mathbf{d}\right)/\left\|\mathbf{a} \times \mathbf{d}\right\|$, as was defined in Section 4.1.1.2.

Note on parameters kf and tp

The parameters kf and tp can be specified either in the Material section or in the *ElementData* section with the tag MRVonMisesParameters. With this second option the user can define different fiber characteristics for each element separately, which can be useful if fiber orientations or concentrations vary spatially. The parameter mat_axis can also be defined either in the Material section or in the *ElementData* section.

Example

This example defines a thin soft tissue material where fibers are distributed according to a constrained von Mises mixture distribution.

```
<material id="1" name="Material 1" type="Mooney-Rivlin von Mises Fibers">
  <c1>10.0</c1>
  <c2>0.0</c2>
  <c3>50.0</c3>
  <c4>5.0</c4>
  <c5>1</c5>
  <lam_max>10</lam_max>
  <k>1000000.0</k>
  <kf>1</kf>
  <vmc>2</vmc>
  <var_n>2.0</var_n>
  <tp>0.0</tp>
  <gipt>40</gipt>
  <mat_axis type="local">4,1,3</mat_axis>
</material>
```

4.1.3 Compressible Materials

Unlike the materials in Section 4.1.2, these materials do not necessarily assume an additive decomposition of the bulk and deviatoric parts of the strain energy or stress. Further, these materials can only be used with the standard displacement-based finite element formulation, rather than the three-field element formulatoin. They should not be used for nearly-incompressible material behavior due to the potential for element locking.

4.1.3.1 Carter-Hayes

The material type for a Carter-Hayes material is *Carter-Hayes*. The following parameters must be defined:

<E0>	Young's modulus at reference density E_0	[**P**]
<rho0>	reference density ρ_0	[**M**/**L**^{3}]
<gamma>	exponent of solid-bound molecule density for calculation of Young's modulus γ	[ ]
<v>	Poisson's ratio ν	[ ]
<sbm>	index of solid bound molecule	[ ]

This model describes a compressible neo-Hookean material [19] whose Young's modulus is a power-law function of the referential apparent density ρ_r^σ of a solid-bound molecule. It is derived from the following hyperelastic strain-energy function:

$$\Psi_r = \frac{E_Y}{2\left(1+\nu\right)}\left[\frac{1}{2}\left(\operatorname{tr}\mathbf{C}-3\right)-\ln J+\frac{\nu}{1-2\nu}\left(\ln J\right)^2\right].$$

Here, $\mathbf{C}$ is the right Cauchy-Green deformation tensor and J is the determinant of the deformation gradient tensor.

Young's modulus depends on ρ_r^σ according to a power law [20, 21],

$$E_Y = E_0\left(\frac{\rho_r^\sigma}{\rho_0}\right)^\gamma.$$

This type of material references a solid-bound molecule that belongs to a multiphasic mixture. Therefore this material may only be used as the solid (or a component of the solid) in a multiphasic mixture (Section 4.9). The solid-bound molecule must be defined in the <Globals> section (Section 3.4.3) and must be included in the multiphasic mixture using a <solid_bound> tag. The parameter *sbm* must refer to the global index of that solid-bound molecule. The value of ρ_r^σ is specified within the <solid_bound> tag. If a chemical reaction is defined within that multiphasic mixture that alters the value of ρ_r^σ, lower and upper bounds may be specified for this referential density within the <solid_bound> tag to prevent E_Y from reducing to zero or achieving excessively elevated values.

Example:

```
<material id="1" name="solid matrix" type="multiphasic">
  <phi0>0</phi0>
  <solid_bound sbm="1">
    <rho0>1</rho0>
```

```
      <rhomin>0.1</rhomin>
      <rhomax>5</rhomax>
    </solid_bound>
    <fixed_charge_density>0</fixed_charge_density>
    <solid type="Carter-Hayes">
      <sbm>1</sbm>
      <E0>10000</E0>
      <rho0>1</rho0>
      <gamma>2.0</gamma>
      <v>0</v>
    </solid>
    <permeability type="perm-const-iso">
      <perm>1</perm>
    </permeability>
    <osmotic_coefficient type="osm-coef-const">
      <osmcoef>1</osmcoef>
    </osmotic_coefficient>
    <reaction name="solid remodeling" type="mass-action-forward">
      <Vbar>0</Vbar>
      <vP sbm="1">1</vP>
      <forward_rate type="Huiskes reaction rate">
        <B>1</B>
        <psi0>0.01</psi0>
      </forward_rate>
    </reaction>
  </material>
```

4.1.3.2 Cell Growth

The material type for cell growth is "*cell growth*" [13]. The following material parameters need to be defined:

<phir>	intracellular solid volume fraction in reference (strain-free) configuration, φ_r^s	[ ]
<cr>	intracellular molar content of membrane-impermeant solute (moles per volume of the cell in the reference configuration), c_r	[**n**/**L**^{3}]
<ce>	extracellular osmolarity, c_e	[**n**/**L**^{3}]

The Cauchy stress for this material is

$$\boldsymbol{\sigma} = -\pi \mathbf{I},$$

where π is the osmotic pressure, given by

$$\pi = RT\left(\frac{c_r}{J-\varphi_r^s} - c_e\right),$$

where $J = \det \mathbf{F}$ is the relative volume. The values of the universal gas constant R and absolute temperature T must be specified as global constants.

Cell growth may be modeled by simply increasing the mass of the intracellular solid matrix and membrane-impermeant solute. This is achieved by allowing the parameters φ_r^s and c_r to increase over time as a result of growth, by associating them with user-defined load curves. Since cell growth is often accompanied by cell division, and since daughter cells typically achieve the same solid and solute content as their parent, it may be convenient to assume that φ_r^s and c_r increase proportionally, though this is not an obligatory relationship. To ensure that the initial configuration is a stress-free reference configuration, let $c_r = (1-\varphi_r^s)\, c_e$ in the initial state prior to growth.

Example (using units of mm, N, s, nmol, K):

```
<Globals>
  <Constants>
    <T>298</T>
    <R>8.314e-06</R>
    <Fc>0</Fc>
  </Constants>
</Globals>
<Material>
  <material id="1" name="Cell" type="cell growth">
    <phir lc="1">1</phir>
    <cr lc="2">1</cr>
    <ce>300</ce>
  </material>
</Material>
<LoadData>
  <loadcurve id="1" type="smooth">
```

```
      <loadpoint>0,0.3</loadpoint>
      <loadpoint>1,0.6</loadpoint>
    </loadcurve>
    <loadcurve id="2" type="smooth">
      <loadpoint>0,210</loadpoint>
      <loadpoint>1,420</loadpoint>
    </loadcurve>
  </LoadData>
```

4.1.3.3 Cubic CLE

The material type for a conewise linear elastic (CLE) material with cubic symmetry is *cubic CLE*. The following parameters must be defined:

<lp1>	Tensile diagonal first Lamé coefficient λ_{+1}	[**P**]
<lm1>	Compressive diagonal first Lamé coefficient λ_{-1}	[**P**]
<l2>	Off-diagonal first Lamé coefficient λ_2	[**P**]
<mu>	Second Lamé coefficient μ	[**P**]

This bimodular elastic material is specialized from the orthotropic conewise linear elastic material described by Curnier et al. [25], to the case of cubic symmetry. It is derived from the following hyperelastic strain-energy function:

$$\Psi_r = \mu \mathbf{I} : \mathbf{E}^2 + \sum_{a=1}^{3} \frac{1}{2} \lambda_1 \left[\mathbf{A}_a^r : \mathbf{E} \right] \left(\mathbf{A}_a^r : \mathbf{E} \right)^2 + \frac{1}{2} \lambda_2 \sum_{\substack{b=1 \\ b \neq a}}^{3} \left(\mathbf{A}_a^r : \mathbf{E} \right) \left(\mathbf{A}_b^r : \mathbf{E} \right) ,$$

where

$$\lambda_1 \left[\mathbf{A}_a^r : \mathbf{E} \right] = \begin{cases} \lambda_{+1} & \mathbf{A}_a^r : \mathbf{E} \geqslant 0 \\ \lambda_{-1} & \mathbf{A}_a^r : \ .E < 0 \end{cases}$$

Here, $\mathbf{E}$ is the Lagrangian strain tensor and $\mathbf{A}_a^r = \mathbf{a}_a^r \otimes \mathbf{a}_a^r$, where $\mathbf{a}_a^r$ ($a = 1, 2, 3$) are orthonormal vectors aligned with the material axes. This material response was originally formulated for infinitesimal strain analyses; its behavior under finite strains may not be physically realistic.

Example:

```
<material id="1" type="cubic CLE">
  <density>1</density>
  <lp1>13.01</lp1>
  <lm1>0.49</lm1>
  <l2>0.66</l2>
  <mu>0.16</mu>
</material>
```

4.1.3.4 Donnan Equilibrium Swelling

The material type for a Donnan equilibrium swelling pressure is "*Donnan equilibrium*". The swelling pressure is described by the equations for ideal Donnan equilibrium, assuming that the material is porous, with a charged solid matrix, and the external bathing environment consists of a salt solution of monovalent counter-ions [45, 37]. Since osmotic swelling must be resisted by a solid matrix, this material is not stable on its own. It must be combined with an elastic material that resists the swelling, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<phiw0>	gel porosity (fluid volume fraction) in reference (strain-free) configuration, φ_0^w	[ ]
<cF0>	fixed-charge density in reference (strain-free) configuration, c_0^F	[**n**/**L**^{3}]
<bosm>	external bath osmolarity, $\bar{c}^*$	[**n**/**L**^{3}]
<Phi>	osmotic coefficient, Φ	[]

The Cauchy stress for this material is the stress from the Donnan equilibrium response [5]:

$$\boldsymbol{\sigma} = -\pi \mathbf{I},$$

where π is the osmotic pressure, given by

$$\pi = RT\Phi\left(\sqrt{(c^F)^2 + (\bar{c}^*)^2} - \bar{c}^*\right),$$

and c^F is the fixed-charge density in the current configuration, related to the reference configuration via

$$c^F = \frac{\varphi_0^w}{J - 1 + \varphi_0^w} c_0^F,$$

where $J = \det \mathbf{F}$ is the relative volume. The values of the universal gas constant R and absolute temperature T must be specified as global constants. For ideal Donnan law, use $\Phi = 1$.

Note that c_0^F may be negative or positive; the gel porosity is unitless and must be in the range $0 < \varphi_0^w < 1$. A self-consistent set of units must be used for this model. For example:

	(m, N, s, mol, K)	(mm, N, s, nmol, K)
R	8.314 J/mol·K	8.314×10^{-6} mJ/nmol·K
T	K	K
c_0^F	Eq/m^3= mEq/L	nEq/mm^3= mEq/L
$\bar{c}^*$	mol/m^3= mM	nmol/mm^3= mM
ξ_i	Pa	MPa
π	Pa	MPa

Though this material is porous, this is not a full-fledged biphasic material as described in Section 4.7 for example. The behavior described by this material is strictly valid only after the transient response of interstitial fluid and ion fluxes has subsided (thus Donnan *equilibrium*).

Donnan osmotic swelling reduces to zero when either $c_0^F = 0$ or $\bar{c}^* \to \infty$. Therefore, entering any other values for c_0^F and $\bar{c}^*$ at the initial time point of an analysis produces an instantaneous, non-zero swelling pressure. Depending on the magnitude of this pressure relative to the solid

matrix stiffness, the nonlinear analysis may not converge due to this sudden swelling. Therefore, it is recommended to prescribe a load curve for either <cF0> or <bosm>, to ease into the initial swelling prior to the application of other loading conditions.

Example (using units of mm, N, s, nmol, K):

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Donnan equilibrium">
    <phiw0>0.8</ phiw0>
    <cF0 lc="1">1</cF0>
    <bosm>300</bosm>
  </solid>
  <solid type="ellipsoidal fiber distribution">
    <ksi>0.01,0.01,0.01</ksi>
    <beta>3,3,3</beta>
  </solid>
</material>
<LoadData>
  <loadcurve id="1">
    <loadpoint>0,0</loadpoint>
    <loadpoint>1,150</loadpoint>
  </loadcurve>
</LoadData>
<Globals>
  <Constants>
    <R>8.314e-6</R>
    <T>310</T>
  </Constants>
</Globals>
```

4.1.3.5 Ellipsoidal Fiber Distribution

The material type for an ellipsoidal continuous fiber distribution is "*ellipsoidal fiber distribution*". Since fibers can only sustain tension, this material is not stable on its own. It must be combined with a stable compressible material that acts as a ground matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<beta>	parameters $(\beta_1, \beta_2, \beta_3)$	[ ]
<ksi>	parameters (ξ_1, ξ_2, ξ_3)	[**P**]

The Cauchy stress for this fibrous material is given by [38, 3, 5]:

$$\boldsymbol{\sigma} = \int_0^{2\pi} \int_0^{\pi} H\left(I_n - 1\right) \sigma_n\left(\mathbf{n}\right) \sin\varphi \, d\varphi \, d\theta.$$

Here, $I_n = \lambda_n^2 = \mathbf{N} \cdot \mathbf{C} \cdot \mathbf{N}$ is the square of the fiber stretch λ_n, $\mathbf{N}$ is the unit vector along the fiber direction, in the reference configuration, which in spherical angles is directed along (θ, φ), $\mathbf{n} = \mathbf{F} \cdot \mathbf{N}/\lambda_n$, and $H\left(.\right)$is the unit step function that enforces the tension-only contribution.

The fiber stress is determined from a fiber strain energy function,

$$\sigma_n = \frac{2I_n}{J} \frac{\partial \Psi}{\partial I_n} \mathbf{n} \otimes \mathbf{n},$$

where in this material,

$$\Psi\left(\mathbf{n}, I_n\right) = \xi\left(\mathbf{n}\right)\left(I_n - 1\right)^{\beta(\mathbf{n})}.$$

The materials parameters $\beta$and $\xi$are assumed to vary ellipsoidally with $\mathbf{n}$, according to

$$\xi\left(\mathbf{n}\right) = \left(\frac{\cos^2\theta \sin^2\varphi}{\xi_1^2} + \frac{\sin^2\theta \sin^2\varphi}{\xi_2^2} + \frac{\cos^2\varphi}{\xi_3^2}\right)^{-1/2}$$
$$\beta\left(\mathbf{n}\right) = \left(\frac{\cos^2\theta \sin^2\varphi}{\beta_1^2} + \frac{\sin^2\theta \sin^2\varphi}{\beta_2^2} + \frac{\cos^2\varphi}{\beta_3^2}\right)^{-1/2}.$$

The orientation of the material axis can be defined as explained in detail in Section 4.1.1.

Example:

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1000.0</E>
    <v>0.45</v>
  </solid>
  <solid type="ellipsoidal fiber distribution">
    <ksi>10, 12, 15</ksi>
    <beta>2.5, 3, 3</beta>
  </solid>
</material>
```

4.1.3.6 Ellipsoidal Fiber Distribution Neo-Hookean

The material type for a Neo-Hookean material with an ellipsoidal continuous fiber distribution is "*EFD neo-Hookean*". The following material parameters need to be defined:

<E>	Young's modulus	[**P**]
<v>	Poisson's ratio	[ ]
<beta>	parameters $(\beta_1, \beta_2, \beta_3)$	[ ]
<ksi>	parameters (ξ_1, ξ_2, ξ_3)	[**P**]

The Cauchy stress for this material is given by,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{NH} + \boldsymbol{\sigma}_f.$$

Here, $\boldsymbol{\sigma}_{NH}$ is the stress from the Neo-Hookean basis (Section 4.1.3.17), and $\boldsymbol{\sigma}_f$ is the stress contribution from the fibers (Section 4.1.3.5).

Example:

```
<material id="1" type="EFD neo-Hookean">
  <E>1</E>
  <v>0.3</v>
  <beta>4.5,4.5,4.5</beta>
  <ksi>1,1,1</ksi>
  <mat_axis type="local">0,0,0</mat_axis>
</material>
```

4.1.3.7 Ellipsoidal Fiber Distribution with Donnan Equilibrium Swelling

The material type for a swelling pressure combined with an ellipsoidal continuous fiber distribution is "*EFD Donnan equilibrium*". The swelling pressure is described by the equations for ideal Donnan equilibrium, assuming that the material is porous, with a charged solid matrix, and the external bathing environment consists of a salt solution of monovalent counter-ions. The following material parameters need to be defined:

<phiw0>	gel porosity (fluid volume fraction) in reference (strain-free) configuration, φ_0^w	[ ]
<cF0>	fixed-charge density in reference (strain-free) configuration, c_0^F	[**n**/**L**^{3}]
<bosm>	external bath osmolarity, $\overline{c}^*$	[**n**/**L**^{3}]
<beta>	parameters $(\beta_1, \beta_2, \beta_3)$	[ ]
<ksi>	parameters (ξ_1, ξ_2, ξ_3)	[**P**]

The Cauchy stress for this material is given by,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{DE} + \boldsymbol{\sigma}_f \,.$$

$\boldsymbol{\sigma}_f$ is the stress contribution from the fibers, as described in Section 4.1.1. $\boldsymbol{\sigma}_{DE}$ is the stress from the Donnan equilibrium response, as described in Section 4.1.3.4

Example (using units of mm, N, s, nmol, K):

```
<material id="1" type="EFD Donnan equilibrium">
  <phiw0>0.8</ phiw0>
  <cF0 lc="1">1</cF0>
  <bosm>300</bosm>
  <beta>3,3,3</beta>
  <ksi>0.01,0.01,0.01</ksi>
  <mat_axis type="local">0,0,0</mat_axis>
</material>
<LoadData>
  <loadcurve id="1">
    <loadpoint>0,0</loadpoint>
    <loadpoint>1,150</loadpoint>
  </loadcurve>
</LoadData>
<Globals>
  <Constants>
    <R>8.314e-6</R>
    <T>310</T>
  </Constants>
</Globals>
```

4.1.3.8 Fiber with Exponential-Power Law

The material type for a single fiber with an exponential-power law is "*fiber-exp-pow*". Since fibers can only sustain tension, this material is not stable on its own. It must be combined with a stable compressible material that acts as a ground matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<ksi>	ξ, representing a measure of the fiber modulus	[**P**]
<alpha>	α, coefficient of exponential argument	[ ]
<beta>	β, power of exponential argument	[ ]

The fiber is oriented along the unit vector $\mathbf{e}_1$, where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are orthonormal basis vectors representing the local element coordinate system when specified (Section 4.1.1), or else the global Cartesian coordinate system. The Cauchy stress for this fibrous material is given by

$$\boldsymbol{\sigma} = H\left(I_n - 1\right) \frac{2I_n}{J} \frac{\partial \Psi}{\partial I_n} \mathbf{n} \otimes \mathbf{n},$$

where $I_n = \lambda_n^2 = \mathbf{N} \cdot \mathbf{C} \cdot \mathbf{N}$ is the square of the fiber stretch, $\mathbf{n} = \mathbf{F} \cdot \mathbf{N}/\lambda_n$, and $H\left(.\right)$ is the unit step function that enforces the tension-only contribution. The fiber strain energy density is given by

$$\Psi = \frac{\xi}{\alpha\beta} \left(\exp\left[\alpha \left(I_n - 1\right)^{\beta}\right] - 1 \right),$$

where $\xi > 0$, $\alpha \geqslant 0$, and $\beta \geqslant 2$.

Note: In the limit when $\alpha \to 0$, this expressions produces a power law,

$$\lim_{\alpha \to 0} \Psi = \frac{\xi}{\beta} \left(I_n - 1\right)^{\beta}$$

Note: When $\beta > 2$, the fiber modulus is zero at the strain origin ($I_n = 1$). Therefore, use $\beta > 2$ when a smooth transition in the stress is desired from compression to tension.

Example:

Single fiber oriented along $\mathbf{e}_1$, embedded in a neo-Hookean ground matrix.

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1000.0</E>
    <v>0.45</v>
  </solid>
  <solid type="fiber-exp-pow">
    <ksi>5</ksi>
    <alpha>20</alpha>
    <beta>3</beta>
    <mat_axis type="angles">
        <theta>0</theta>
        <phi>90</phi>
    </mat_axis>
  </solid>
</material>
```

Example:

Two fibers in the plane orthogonal to $\mathbf{e}_1$, oriented at ±25 degrees relative to $\mathbf{e}_3$, embedded in a neo-Hookean ground matrix.

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1000.0</E>
    <v>0.45</v>
  </solid>
  <solid type="fiber-exp-pow"
<ksi>5</ksi>
<alpha>20</alpha>
<beta>3</beta>
<mat_axis type="angles">
  <theta>90</theta>
  <phi>25</phi>
</mat_axis>
</solid>
<solid type="fiber-exp-pow">
  <ksi>5</ksi>
  <alpha>20</alpha>
  <beta>3</beta>
  <mat_axis type="angles">
    <theta>-90</theta>
    <phi>25</phi>
  </mat_axis>
</solid>
</material>
```

4.1.3.9 Fiber with Toe-Linear Response

This material type is "*fiber-pow-linear*". The following material parameters need to be defined:

<E>	E, the fiber modulus in the linear range ($E \geqslant 0$)	[**P**]
<beta>	β, the power-law exponent in the toe region ($\beta \geqslant 2$)	[ ]
<lam0>	λ_0, the stretch ratio when the toe region transitions to the linear region ($\lambda_0 > 1$)	[ ]

The fiber strain energy density is given by

$$\Psi_n\left(I_n\right) = \begin{cases} 0 & I_n < 1 \\ \frac{\xi}{2\beta}\left(I_n - 1\right)^{\beta} & 1 \leqslant I_n \leqslant I_0 \\ E\left(I_0^{1/2} - I_n^{1/2}\right) + B\left(I_n - I_0\right) + \Psi_0 & I_0 < I_n \end{cases},$$

where $I_0 = \lambda_0^2$,

$$\xi = \frac{E}{2\left(\beta - 1\right)}\left(I_0 - 1\right)^{2-\beta},\ B = \frac{E}{2}\left[\frac{\left(I_0 - 1\right)}{2\left(\beta - 1\right)} + I_0\right],\ \Psi_0 = \frac{\xi}{2\beta}\left(I_0 - 1\right)^{\beta}$$

Example:

```
<material type="fiber-power-linear">
  <fiber type="angles">
    <theta>20</center>
    <phi>90</phi>
  </fiber>
  <E>1</E>
  <beta>2.5</beta>
  <lam0>1.06</lam0>
</material>
```

4.1.3.10 Fung Orthotropic Compressible

The material type for unconstrained orthotropic Fung elasticity [27, 26] is "*Fung-ortho-compressible*". The following material parameters must be defined:

<E1>	E_1 Young's modulus	[**P**]
<E2>	E_2 Young's modulus	[**P**]
<E3>	E_3 Young's modulus	[**P**]
<G12>	G_{12} shear modulus	[**P**]
<G23>	G_{23} shear modulus	[**P**]
<G31>	G_{31} shear modulus	[**P**]
<v12>	ν_{12} Poisson's ratio	[ ]
<v23>	ν_{23} Poisson's ratio	[ ]
<v31>	ν_{31} Poisson's ratio	[ ]
<c>	c coefficient	[**P**]
<k>	κ bulk modulus	[**P**]

The hyperelastic strain energy function is given by [4],

$$\Psi = \frac{1}{2}c\left(e^{Q}-1\right)+U\left(J\right),$$

where,

$$Q = c^{-1}\sum_{a=1}^{3}\left[2\mu_a\mathbf{M}_a:\mathbf{E}^2+\sum_{b=1}^{3}\lambda_{ab}\left(\mathbf{M}_a:\mathbf{E}\right)\left(\mathbf{M}_b:\mathbf{E}\right)\right],$$

and

$$U\left(J\right) = \frac{\kappa}{2}\left(\ln J\right)^2 .$$

Here, $\mathbf{E} = \left(\mathbf{C}-\mathbf{I}\right)/2$ and $\mathbf{M}_a = \mathbf{V}_a \otimes \mathbf{V}_a$where $\mathbf{V}_a$ defines the initial direction of material axis a. See Section 4.1.1.2 on how to define the material axes for orthotropic materials. The Lamé constants μ_a $(a = 1, 2, 3)$ and λ_{ab} $(a, b = 1, 2, 3,\ \lambda_{ba} = \lambda_{ab})$ are related to Young's moduli E_a, shear moduli G_{ab} and Poisson's ratios ν_{ab} via

$$\begin{bmatrix} \lambda_{11}+2\mu_1 & \lambda_{12} & \lambda_{13} & 0 & 0 & 0 \\ \lambda_{12} & \lambda_{22}+2\mu_2 & \lambda_{23} & 0 & 0 & 0 \\ \lambda_{13} & \lambda_{23} & \lambda_{33}+2\mu_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}\left(\mu_1+\mu_2\right) & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}\left(\mu_2+\mu_3\right) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}\left(\mu_1+\mu_3\right) \end{bmatrix}^{-1}$$

$$= \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{12}}{E_1} & -\frac{\nu_{13}}{E_1} & 0 & 0 & 0 \\ -\frac{\nu_{21}}{E_2} & \frac{1}{E_2} & -\frac{\nu_{23}}{E_2} & 0 & 0 & 0 \\ -\frac{\nu_{31}}{E_3} & -\frac{\nu_{32}}{E_3} & \frac{1}{E_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{12}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{23}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{31}} \end{bmatrix}$$

The orthotropic Lamé parameters should produce a positive definite stiffness matrix.

Example:

```
<material id="3" type="Fung-ortho-compressible">
  <E1>124</E1>
  <E2>124</E2>
  <E3>36</E3>
  <G12>67</G12>
  <G23>40</G23>
  <G31>40</G31>
  <v12>-0.075</v12>
  <v23>0.87</v23>
  <v31>0.26</v31>
  <c>1</c>
  <k>120</k>
</material>
```

4.1.3.11 Holmes-Mow

The material type for the Holmes-Mow material [32] is *Holmes-Mow*. This isotropic hyperelastic material has been used to represent the solid matrix of articular cartilage [32, 7] and intervertebral disc [35]. The following material parameters must be defined:

<E>	Young's modulus	[**P**]
<v>	Poisson's ratio	[ ]
<beta>	Exponential stiffening coefficient	[ ]

The coupled hyperelastic strain-energy function for this material is given by [32]:

$$W\left(I_1, I_2, J\right) = \frac{1}{2} c \left(e^Q - 1\right),$$

where I_1 and I_2 are the first and second invariants of the right Cauchy-Green tensor and $J$is the jacobian of the deformation gradient. Furthermore,

$$\begin{aligned} Q &= \frac{\beta}{\lambda + 2\mu}\left[\left(2\mu - \lambda\right)\left(I_1 - 3\right) + \lambda\left(I_2 - 3\right) - \left(\lambda + 2\mu\right)\ln J^2\right] \\ c &= \frac{\lambda + 2\mu}{2\beta} \end{aligned},$$

and λ and μ are the Lamé parameters which are related to the more familiar Young's modulus and Poisson's ratio in the usual manner:

$$\begin{aligned} \lambda &= \frac{E}{\left(1+\nu\right)\left(1-2\nu\right)} \\ \mu &= \frac{E}{2\left(1+\nu\right)} \end{aligned}.$$

Example:

```
<material id="3" type="Holmes-Mow">
  <E>1</E>
  <v>0.35</v>
  <beta>0.25</beta>
</material>
```

4.1.3.12 Isotropic Elastic

The material type for isotropic elasticity is *isotropic elastic*[1]. The following material parameters must be defined:

<E>	Young's modulus	[**P**]
<v>	Poisson's ratio	[ ]

This material is an implementation of a hyperelastic constitutive material that reduces to the classical linear elastic material for small strains, but is objective for large deformations and rotations. The hyperelastic strain-energy function is given by:

$$W = \frac{1}{2}\lambda \left(\operatorname{tr} \mathbf{E}\right)^2 + \mu \mathbf{E} : \mathbf{E}.$$

Here, $\mathbf{E}$ is the Euler-Lagrange strain tensor and λ and μ are the Lamé parameters, which are related to the more familiar Young's modulus E and Poisson's ratio ν as follows:

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}, \mu = \frac{E}{2(1+\nu)}.$$

It is often convenient to express the material properties using the bulk modulus K and shear modulus G. To convert to Young's modulus and Poisson's ratio, use the following formulas:

$$E = \frac{9KG}{3K+G}, \quad \nu = \frac{3K-2G}{6K+2G}.$$

Remark: Note that although this material is objective, it is not advised to use this model for large strains since the behavior may be unphysical. For example, it can be shown that for a uniaxial tension the stress grows unbounded and the volume tends to zero for finite strains. Also for large strains, the Young's modulus and Poisson's ratio input values have little relationship to the actual material parameters. Therefore it is advisable to use this material only for small strains and/or large rotations. To represent isotropic elastic materials under large strain and rotation, it is best to use some of the other available nonlinear material models described in this chapter, such as the Holmes-Mow material in Section 4.1.3.11, the neo-Hookean material in Section 4.1.3.17, or the unconstrained Ogden material in Section 4.1.3.20.

Example:

```
<material id="1" type="isotropic elastic"
  <E>1000.0</E>
  <v>0.45</v>
</material>
```

[1] This material replaces the now-obsolete *linear elastic* and *St.Venant-Kirchhoff* materials. These materials are still available for backward compatibility although it is recommended to use the *isotropic elastic* material instead.

4.1.3.13 Orthotropic Elastic

The material type for orthotropic elasticity is "*orthotropic elastic*". The following material parameters must be defined:

<E1>	Young's modulus in the x-direction	[**P**]
<E2>	Young's modulus in the y-direction	[**P**]
<E3>	Young's modulus in the z-direction	[**P**]
<G12>	Shear modulus in the xy-plane	[**P**]
<G23>	Shear modulus in the yz-plane	[**P**]
<G31>	Shear modulus in the xz-plane	[**P**]
<v12>	Poisson's ratio between x- and y-direction	[ ]
<v23>	Poisson's ratio between y- and z-direction	[ ]
<v31>	Poisson's ratio between z- and x-direction	[ ]

The stress-strain relation for this material is given by

$$\begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{23} \\ 2E_{31} \\ 2E_{12} \end{bmatrix} = \begin{bmatrix} 1/E_1 & -\nu_{21}/E_2 & -\nu_{31}/E_3 & 0 & 0 & 0 \\ -\nu_{12}/E_1 & 1/E_2 & -\nu_{32}/E_3 & 0 & 0 & 0 \\ -\nu_{13}/E_1 & -\nu_{23}/E_2 & 1/E_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{23} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{31} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{12} \end{bmatrix} \begin{bmatrix} T_{11} \\ T_{22} \\ T_{33} \\ T_{23} \\ T_{31} \\ T_{12} \end{bmatrix}$$

Material axes may be specified as described in Section 4.1.1.2.

Example:

```
<material id="3" type="orthotropic elastic">
  <mat_axis type="vector">
    <a>0.866,0.5,0</a>
    <d>-0.5,0.866,0</d>
  </mat_axis>
  <E1>1</E1>
  <E2>2</E2>
  <E3>3</E3>
  <v12>0</v12>
  <v23>0</v23>
  <v31>0</v31>
  <G12>1</G12>
  <G23>1</G23>
  <G31>1</G31>
</material>
```

4.1.3.14 Orthotropic CLE

The material type for a conewise linear elastic (CLE) material with orthtropic symmetry is *orthotropic CLE*. The following parameters must be defined:

<lp11>	Tensile diagonal first Lamé coefficient along direction 1 λ_{+11}	[P]
<lp22>	Tensile diagonal first Lamé coefficient along direction 2 λ_{+22}	[P]
<lp11>	Tensile diagonal first Lamé coefficient along direction 3 λ_{+33}	[P]
<lm11>	Compressive diagonal first Lamé coefficient along direction 1 λ_{-11}	[P]
<lm22>	Compressive diagonal first Lamé coefficient along direction 2 λ_{-22}	[P]
<lm33>	Compressive diagonal first Lamé coefficient along direction 3 λ_{-33}	[P]
<l12>	Off-diagonal first Lamé coefficient in 1-2 plane λ_{12}	[P]
<l23>	Off-diagonal first Lamé coefficient in 2-3 plane λ_{23}	[P]
<l31>	Off-diagonal first Lamé coefficient in 3-1 plane λ_{31}	[P]
<mu1>	Second Lamé coefficient along direction 1 μ_1	[P]
<mu2>	Second Lamé coefficient along direction 2 μ_2	[P]
<mu3>	Second Lamé coefficient along direction 3 μ_3	[P]

This bimodular elastic material is the orthotropic conewise linear elastic material described by Curnier et al. [25]. It is derived from the following hyperelastic strain-energy function:

$$\Psi_r = \sum_{a=1}^{3} \mu_a \mathbf{A}_a^r : \mathbf{E}^2 + \frac{1}{2}\lambda_{aa}\left[\mathbf{A}_a^r : \mathbf{E}\right]\left(\mathbf{A}_a^r : \mathbf{E}\right)^2 + \sum_{\substack{b=1 \\ b \neq a}}^{3} \frac{1}{2}\lambda_{ab}\left(\mathbf{A}_a^r : \mathbf{E}\right)\left(\mathbf{A}_b^r : \mathbf{E}\right)$$

where $\lambda_{ba} = \lambda_{ab}$ and

$$\lambda_{aa}\left[\mathbf{A}_a^r : \mathbf{E}\right] = \begin{cases} \lambda_{+aa} & \mathbf{A}_a^r : \mathbf{E} \geqslant 0 \\ \lambda_{-aa} & \mathbf{A}_a^r : \mathbf{E} < 0 \end{cases}, \quad a = 1, 2, 3$$

Here, $\mathbf{E}$ is the Lagrangian strain tensor and $\mathbf{A}_a^r = \mathbf{a}_a^r \otimes \mathbf{a}_a^r$, where $\mathbf{a}_a^r$ $(a = 1, 2, 3)$ are orthonormal vectors aligned with the material axes. This material response was originally formulated for infinitesimal strain analyses; its behavior under finite strains may not be physically realistic.

Example:

```
<material id="1" type=" orthotropic CLE">
  <density>1</density>
  <lp11>13.01</lp11>
  <lp22>13.01</lp22>
  <lp33>13.01</lp33>
  <lm11>0.49</lm11>
  <lm22>0.49</lm22>
  <lm33>0.49</lm33>
  <l12>0.66</l12>
  <l23>0.66</l23>
  <l31>0.66</l31>
  <mu1>0.16</mu1>
  <mu2>0.16</mu2>
  <mu3>0.16</mu3>
</material>
```

4.1.3.15 Osmotic Pressure from Virial Expansion

The material type for osmotic pressure from virial expansion is "*osmotic virial expansion*". The following material parameters need to be defined:

<phiw0>	Fluid volume fraction in reference (strain-free) configuration, φ_r^w	[ ]
<cr>	Concentration of interstitial solute causing the osmotic pressure (moles per volume of the mixture in the reference configuration), c_r	[**n**/**L**^{3}]
<c1>	First virial coefficient c_1	[**F**·**L**/**n**]
<c2>	Second virial coefficient c_2	[**F**·**L**^{4}/**n**^{2}]
<c3>	Third virial coefficient c_3	[**F**·**L**^{7}/**n**^{3}]

The Cauchy stress for this material is

$$\boldsymbol{\sigma} = -\pi \mathbf{I},$$

where π is the osmotic pressure, given by

$$\pi = c_1 c + c_2 c^2 + c_3 c^3, \quad c = \frac{\varphi_r^w c_r}{J - 1 + \varphi_r^w},$$

c is the solute concentration in the current configuration, and $J = \det \mathbf{F}$ is the relative volume.

This osmotic swelling pressure in the interstitial fluid of a porous material represents an entropic mechanism whose magnitude is independent of the external bath osmolarity. Typically, this material should be used in a solid mixture where the swelling pressure is resisted by a solid matrix in tension.

Example:

```
<Material>
  <material id="1" type="solid mixture">
    <solid type="osmotic virial expansion">
      <phiw0>0.8</phiw0>
      <cr lc="1">100</cr>
      <c1>2.436e-6</c1>
      <c2>0</c2>
      <c3>0</c3>
    </solid>
    <solid type="spherical fiber distribution"/>
  </material>
</Material>
<LoadData>
  <loadcurve id="1" type="smooth">
    <loadpoint>0,0</loadpoint>
    <loadpoint>1,1</loadpoint>
  </loadcurve>
</LoadData>
```

4.1.3.16 Natural Neo-Hookean

The material type for a natural Neo-Hookean material is *natural neo-Hookean*. The following parameters must be defined:

<G>	shear modulus	[**P**]
<k>	bulk modulus	[**P**]

This model describes a compressible Neo-Hookean material using the natural strain tensor [24]. It has a non-linear stress-strain behavior, but reduces to the classical linear elasticity model for small strains *and* small rotations. It is derived from the following hyperelastic strain-energy function:

$$W = \frac{\kappa}{2} K_1^2 + \mu K_2^2.$$

Here, K_1 and K_2 are the first and second invariants of the left natural (Hencky) strain tensor $\boldsymbol{\eta} = \ln \mathbf{V}$ where $\mathbf{V}$ is the left stretch tensor in the polar decomposition $\mathbf{F} = \mathbf{V} \cdot \mathbf{R}$.

This material model uses a standard displacement-based element formulation, so care must be taken when modeling materials with nearly-incompressible material behavior to avoid element locking. For this case, use the *Mooney-Rivlin* material described in Section 4.1.2.8.

Example:

```
<material id="1" type="natural neo-Hookean">
  <G>500.0</G>
  <k>333.3</k>
</material>
```

4.1.3.17 Neo-Hookean

The material type for a Neo-Hookean material is *neo-Hookean*. The following parameters must be defined:

<E>	Young's modulus	[**P**]
<v>	Poisson's ratio	[ ]

This model describes a compressible Neo-Hookean material [19]. It has a non-linear stress-strain behavior, but reduces to the classical linear elasticity model for small strains *and* small rotations. It is derived from the following hyperelastic strain-energy function:

$$W = \frac{\mu}{2}\left(I_1 - 3\right) - \mu \ln J + \frac{\lambda}{2}\left(\ln J\right)^2 .$$

Here, I_1 and I_2 are the first and second invariants of the right Cauchy-Green deformation tensor $\mathbf{C}$ and J is the determinant of the deformation gradient tensor.

This material model uses a standard displacement-based element formulation, so care must be taken when modeling materials with nearly-incompressible material behavior to avoid element locking. For this case, use the *Mooney-Rivlin* material described in Section 4.1.2.8.

Example:

```
<material id="1" type="neo-Hookean">
  <E>1000.0</E>
  <v>0.45</v>
</material>
```

4.1.3.18 Coupled Mooney-Rivlin

The coupled Mooney-Rivlin material describes a compressible formulation of the Mooney-Rivlin material. The material type for this material is *coupled Mooney-Rivlin*. The following material parameters can be defined.

<c1>	Mooney-Rivlin c1 parameter	[**P**]
<c2>	Mooney-Rivlin c2 parameter	[**P**]
k	"Bulk-modulus"	[**P**]

The strain-energy function is given by the following expression.

$$W = c_1 (I_1 - 3) + c_2 (I_2 - 3) - 2 (c_1 + 2c_2) \ln J + \frac{\lambda}{2} (\ln J)^2$$

Here, I_1 and I_2 are the first and second invariants of the right Cauchy-Green deformation tensor $\mathbf{C}$ and J is the determinant of the deformation gradient tensor.

This material model uses a standard displacement-based element formulation, so care must be taken when modeling materials with nearly-incompressible material behavior to avoid element locking. For (nearly-) incompressible materials, use the *Mooney-Rivlin* material described in Section 4.1.2.8.

Example:

```
<material id="1" type="coupled Mooney-Rivlin">
  <c1>10.0</c1>
  <c2>1.0</c2>
  <k>100.0</k>
</material>
```

4.1.3.19 Coupled Veronda-Westmann

The material type for the coupled Veronda-Westmann material is *coupled Veronda-Westmann*. The following material parameters can be defined.

<c1>	Veronda-Westmann c1 parameter	[**P**]
<c2>	Veronda-Westmann c2 parameter	[**P**]
k	"Bulk-modulus"	[**P**]

The coupled Veronda-Westmann material is a compressible formulation of the Veronda-Westmann material and is defined by the following strain-energy function.

$$W = c_1 \left(e^{c_2 (I_1 - 3)} - 1 \right) - \frac{c_1 c_2}{2} (I_2 - 3) + \frac{\lambda}{2} (\ln J)^2$$

Here, I_1 and I_2 are the first and second invariants of the right Cauchy-Green deformation tensor **C** and $J$is the determinant of the deformation gradient tensor.

This material model uses a standard displacement-based element formulation, so care must be taken when modeling materials with nearly-incompressible material behavior to avoid element locking. For (nearly-) incompressible materials, use the *Veronda-Westmann* material described in Section 4.1.2.16.

Example:

```
<material id="1" type="coupled Veronda-Westmann">
  <c1>10.0</c1>
  <c2>1.0</c2>
  <k>100.0</k>
</material>
```

4.1.3.20 Ogden Unconstrained

This material describes a compressible (unconstrained) hyperelastic Ogden material [51]. The following material parameters must be defined:

<c[n]>	Coefficient of n^{th} term, where n can range from 1 to 6	[**P**]
<m[n]>	Exponent of n^{th} term, where n can range from 1 to 6	[ ]
<cp>	Bulk-like modulus	[**P**]

The hyperelastic strain energy function for this material is given in terms of the eigenvalues of the right or left stretch tensor:

$$W(\lambda_1, \lambda_2, \lambda_3) = \frac{1}{2} c_p (J-1)^2 + \sum_{i=1}^{N} \frac{c_i}{m_i^2} \left(\lambda_1^{m_i} + \lambda_2^{m_i} + \lambda_3^{m_i} - 3 - m_i \ln J\right).$$

Here, λ_i^2 are the eigenvalues of the right or left Cauchy deformation tensor, c_p, c_i and $m_i$are material coefficients and N ranges from 1 to 6. Any material parameters that are not specified by the user are assumed to be zero.

Example:

```
<material id="1" type="Ogden unconstrained">
  <m1>2.4</m1>
  <c1>1</c1>
  <cp>2</cp>
</material>
```

4.1.3.21 Perfect Osmometer Equilibrium Osmotic Pressure

The material type for a perfect osmometer equilibrium swelling pressure is "*perfect osmometer*". The swelling pressure is described by the equations for a perfect osmometer, assuming that the material is porous, containing an interstitial solution whose solutes cannot be exchanged with the external bathing environment; similarly, solutes in the external bathing solution cannot be exchanged with the interstitial fluid of the porous material. Therefore, osmotic pressurization occurs when there is an imbalance between the interstitial and bathing solution osmolarities. Since osmotic swelling must be resisted by a solid matrix, this material is not stable on its own. It must be combined with an elastic material that resists the swelling, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<phiw0>	gel porosity (fluid volume fraction) in reference (strain-free) configuration, φ_0^w	[ ]
<iosm>	interstitial fluid osmolarity in reference configuration, $\bar{c}_0$	[**n**/**L**^{3}]
<bosm>	external bath osmolarity, $\bar{c}^*$	[**n**/**L**^{3}]

The Cauchy stress for this material is the stress from the perfect osmometer equilibrium response:

$$\boldsymbol{\sigma} = -\pi \mathbf{I},$$

where π is the osmotic pressure, given by

$$\pi = RT\left(\bar{c} - \bar{c}^*\right) .$$

$\bar{c}$ is the interstitial fluid in the current configuration, related to the reference configuration via

$$\bar{c} = \frac{\varphi_0^w}{J - 1 + \varphi_0^w}\bar{c}_0 ,$$

where $J = \det \mathbf{F}$ is the relative volume. The values of the universal gas constant R and absolute temperature T must be specified as global constants.

Though this material is porous, this is not a full-fledged biphasic material as described in Section 4.7 for example. The behavior described by this material is strictly valid only after the transient response of interstitial fluid and solute fluxes has subsided.

Example (using units of mm, N, s, nmol, K):

Hyperosmotic loading of a cell with a membrane-impermeant solute, starting from isotonic conditions.

```
<material id="1" type="solid mixture">
  <solid type="perfect osmometer">
    <phiw0>0.8</ phiw0>
    <iosm>300</cF0>
    <bosm lc="1">1</bosm>
  </solid>
  <solid type="neo-Hookean">
    <E>1.0</E>
    <v>0</v>
  </solid>
```

```
</material>
<LoadData>
  <loadcurve id="1">
    <loadpoint>0,300</loadpoint>
    <loadpoint>1,1500</loadpoint>
  </loadcurve>
</LoadData>
<Globals>
  <Constants>
    <R>8.314e-6</R>
    <T>310</T>
  </Constants>
</Globals>
```

4.1.3.22 Porous Neo-Hookean

This material describes a porous neo-Hookean material with referential solid volume fraction φ_r^s (i.e., porosity $\varphi_r^w = 1 - \varphi_r^s$). The pores are compressible but the skeleton is intrinsically incompressible. Thus, upon pore closure, the material behavior needs to switch from compressible to incompressible. This material may be used to model the porous solid matrix of a biphasic or multiphasic material.

The material type for a porous Neo-Hookean material is *porous neo-Hookean*. The following parameters must be defined:

<E>	Young's modulus	[**P**]
<phi0>	Referential solid volume fraction ($0 \leq \varphi_r^s < 1$)	[ ]

This model is derived from the following hyperelastic strain-energy function:

$$W = \frac{\mu}{2}\left(\bar{I}_1 - 3\right) - \mu \ln \bar{J}\,,$$

where $\bar{J}$ represents the pore volume ratio, evaluated from

$$\bar{J} = \frac{J - \varphi_r^s}{1 - \varphi_r^s}\,,$$

and $\bar{I}_1 = \mathrm{tr}\bar{\mathbf{C}}$, with

$$\bar{\mathbf{F}} = \left(\frac{\bar{J}}{J}\right)^{1/3}\mathbf{F}\,, \quad \bar{\mathbf{C}} = \bar{\mathbf{F}}^T \cdot \bar{\mathbf{F}} = \left(\frac{\bar{J}}{J}\right)^{2/3}\mathbf{C}\,,$$

and $\bar{J} = \det \bar{\mathbf{F}}$. The porosity φ^w in the current configuration evolves with the volume ratio J according to

$$\varphi^w = \frac{J - 1 + \varphi_r^w}{J} = \frac{J - \varphi_r^s}{J} = \bar{J}\left(1 - \varphi_r^s\right)\,.$$

Thus, pore closure occurs when $J = \varphi_r^s$ and $\bar{J} = 0$.

By comparison to a standard neo-Hookean material, this porous neo-Hookean material has an effective Young's modulus equal to

$$E = \frac{3\mu}{1 + \frac{1}{2}\left(\varphi_r^w\right)^2}\,,$$

and an effective Poisson's ratio equal to

$$\nu = \frac{1 - \left(\varphi_r^w\right)^2}{2 + \left(\varphi_r^w\right)^2}\,.$$

Therefore, the two material properties that need to be provided are E and the referential porosity $\varphi_r^s = 1 - \varphi_r^w$. Poisson's ratio in the limit of infinitesimal strains is dictated by the porosity according to the above formula. In particular, a highly porous material ($\varphi_r^w \to 1$) has an effective Poisson ratio that approaches zero ($\nu \to 0$) and $E \to 2\mu$ in the range of infinitesimal strains. A low porosity material ($\varphi_r^w \to 0$) has $\nu \to \frac{1}{2}$ and $E \to 3\mu$, which is the expected behavior of an incompressible neo-Hookean solid. Note that setting $\varphi_r^w = 0$ ($\varphi_r^s = 1$) would not produce good numerical behavior, since the Cauchy stress in an incompressible material would need to be supplemented by a hydrostatic pressure term (a Lagrange multiplier that enforces the incompressibility constraint). Nevertheless, this compressible porous neo-Hookean material behaves well even for values of φ^w as low as ~ 0.015.

Example:

```
<material id="1" type="porous neo-Hookean">
  <density>1.0</density>
  <E>1.0</E>
  <phi0>0.2</phi0>
</material>
```

4.1.3.23 Solid Mixture

This material describes a mixture of compressible elastic solids. It is a container for any combination of the materials described in Section 4.1.3.

<solid>	Container tag for compressible material

The mixture may consist of any number of solids. The stress tensor for the solid mixture is the sum of the stresses for all the solids.

Material axes may be optionally specified within the <material> level, as well as within each <solid>. Within the <material> level, these represent the local element axes relative to the global coordinate system. Within the <solid>, they represent local material axes relative to the element. If material axes are specified at both levels, they are properly compounded to produce local material axes relative to the global coordinate system. Material axes specified in the <ElementData> section are equivalent to a specification at the <material> level: they correspond to local element axes relative to the global system.

Example:

```
<material id="1" type="solid mixture">
  <solid type="neo-Hookean">
    <E>1000.0</E>
    <v>0.45</v>
  </solid>
  <solid type="ellipsoidal fiber distribution">
    <mat_axis type="vector">
      <a>0.8660254, 0.5, 0</a>
      <d>0,0,1</d>
    </mat_axis>
    <ksi>5, 1, 1</ksi>
    <beta>2.5, 3, 3</beta>
  </solid>
  <solid type="ellipsoidal fiber distribution">
    <mat_axis type="vector">
      <a>0.8660254,-0.5, 0</a>
      <d>0,0,1</d>
    </mat_axis>
    <ksi>5, 1, 1</ksi>
    <beta>2.5, 3, 3</beta>
  </solid>
</material>
```

4.1.3.24 Spherical Fiber Distribution

The material type for a spherical (isotropic) continuous fiber distribution is "*spherical fiber distribution*". Since fibers can only sustain tension, this material is not stable on its own. It must be combined with a stable compressible material that acts as a ground matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<alpha>	parameter α	[ ]
<beta>	parameter β	[ ]
<ksi>	parameters ξ	[**P**]

The Cauchy stress for this fibrous material is given by [38, 3, 5]:

$$\boldsymbol{\sigma} = \int_0^{2\pi} \int_0^{\pi} H\left(I_n - 1\right) \sigma_n\left(\mathbf{n}\right) \sin\varphi \, d\varphi \, d\theta \, .$$

Here, $I_n = \lambda_n^2 = \mathbf{N} \cdot \mathbf{C} \cdot \mathbf{N}$ is the square of the fiber stretch λ_n, $\mathbf{N}$ is the unit vector along the fiber direction, in the reference configuration, which in spherical angles is directed along (θ, φ), $\mathbf{n} = \mathbf{F} \cdot \mathbf{N}/\lambda_n$, and $H\left(.\right)$ is the unit step function that enforces the tension-only contribution.

The fiber stress is determined from a fiber strain energy function,

$$\sigma_n = \frac{2I_n}{J} \frac{\partial \Psi}{\partial I_n} \mathbf{n} \otimes \mathbf{n} \, ,$$

where in this material, the fiber strain energy density is given by

$$\Psi = \frac{\xi}{\alpha} \left(\exp\left[\alpha \left(I_n - 1\right)^{\beta} \right] - 1 \right) \, ,$$

where $\xi > 0$, $\alpha \geqslant 0$, and $\beta \geqslant 2$.

Note: In the limit when $\alpha \to 0$, this expressions produces a power law,

$$\lim_{\alpha \to 0} \Psi = \xi \left(I_n - 1\right)^{\beta}$$

Note: When $\beta > 2$, the fiber modulus is zero at the strain origin ($I_n = 1$). Therefore, use $\beta > 2$ when a smooth transition in the stress is desired from compression to tension.

Example:

```
<material id="1" type="solid mixture">
  <solid type="neo-Hookean">
    <E>1000.0</E>
    <v>0.45</v>
  </solid>
  <solid type="spherical fiber distribution">
    <ksi>10</ksi>
    <alpha>0</alpha>
    <beta>2.5</beta>
  </solid>
</material>
```

4.1.3.25 Spherical Fiber Distribution from Solid-Bound Molecule

The material type for a spherical (isotropic) continuous fiber distribution with fiber modulus dependent on solid-bound molecule content is "*spherical fiber distribution sbm*". Since fibers can only sustain tension, this material is not stable on its own. It must be combined with a stable compressible material that acts as a ground matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<alpha>	parameter α	[ ]
<beta>	parameter β	[ ]
<ksi0>	fiber modulus ξ_0	[**P**]
<gamma>	fiber modulus exponent γ	[ ]
<rho0>	fiber mass density ρ_0	[**M**/**L**^{3}]
sbm	index of solid-bound molecule σ	[ ]

The Cauchy stress for this fibrous material is given by [38, 3, 5]:

$$\boldsymbol{\sigma} = \int_0^{2\pi} \int_0^{\pi} H\left(I_n - 1\right) \sigma_n\left(\mathbf{n}\right) \sin\varphi \, d\varphi \, d\theta \, .$$

Here, $I_n = \lambda_n^2 = \mathbf{N} \cdot \mathbf{C} \cdot \mathbf{N}$ is the square of the fiber stretch λ_n, $\mathbf{N}$ is the unit vector along the fiber direction, in the reference configuration, which in spherical angles is directed along (θ, φ), $\mathbf{n} = \mathbf{F} \cdot \mathbf{N}/\lambda_n$, and $H\left(.\right)$ is the unit step function that enforces the tension-only contribution.

The fiber stress is determined from a fiber strain energy function,

$$\sigma_n = \frac{2I_n}{J} \frac{\partial \Psi}{\partial I_n} \mathbf{n} \otimes \mathbf{n} \, ,$$

where in this material, the fiber strain energy density is given by

$$\Psi = \frac{\xi}{\alpha} \left(\exp\left[\alpha \left(I_n - 1\right)^{\beta} \right] - 1 \right) \, ,$$

where $\xi > 0$, $\alpha \geqslant 0$, and $\beta \geqslant 2$. The fiber modulus is dependent on the solid-bound molecule referential density ρ_r^{σ} according to the power law relation

$$\xi = \xi_0 \left(\frac{\rho_r^{\sigma}}{\rho_0} \right)^{\gamma} \, ,$$

where ρ_0 is the density at which $\xi = \xi_0$.

This type of material references a solid-bound molecule that belongs to a multiphasic mixture. Therefore this material may only be used as the solid (or a component of the solid) in a multiphasic mixture (Section 4.9). The solid-bound molecule must be defined in the <Globals> section (Section 3.4.3) and must be included in the multiphasic mixture using a <solid_bound> tag. The parameter *sbm* must refer to the global index of that solid-bound molecule. The value of ρ_r^{σ} is specified within the <solid_bound> tag. If a chemical reaction is defined within that multiphasic mixture that alters the value of ρ_r^{σ}, lower and upper bounds may be specified for this referential density within the <solid_bound> tag to prevent ξ from reducing to zero or achieving excessively elevated values.

Note: In the limit when $\alpha \to 0$, the expression for Ψ produces a power law,

$$\lim_{\alpha \to 0} \Psi = \xi \left(I_n - 1\right)^{\beta}$$

Note: When $\beta > 2$, the fiber modulus is zero at the strain origin ($I_n = 1$). Therefore, use $\beta > 2$ when a smooth transition in the stress is desired from compression to tension.

Example:

```
<solid type="solid mixture">
  <solid type="neo-Hookean">
    <E>1000.0</E>
    <v>0.45</v>
  </solid>
  <solid type="spherical fiber distribution sbm">
    <alpha>0</alpha>
    <beta>2.5</beta>
    <ksi0>10</ksi0>
    <gamma>2</gamma>
    <rho0>1</rho0>
    <sbm>1</sbm>
  </solid>
</solid>
```

4.1.3.26 Coupled Transversely Isotropic Mooney-Rivlin

This material describes a transversely isotropic Mooney-Rivlin material using a fully-coupled formulation. It is define through the *coupled trans-iso Mooney-Rivlin* material type. The following material parameters must be defined.

c1	Mooney-Rivlin c_1 parameter.	[**P**]
c2	Mooney-Rivlin c_2 parameter.	[**P**]
c3	exponential multiplier	[**P**]
c4	fiber scale factor	[ ]
c5	fiber modulus in linear region	[**P**]
lam_max	maximum fiber straightening stretch	[ ]
k	bulk-like modulus	[**P**]

The strain-energy function for this constitutive model is defined by

$$W = c_1 (I_1 - 3) + c_2 (I_2 - 3) - 2 (c_1 + 2c_2) \ln J + F(\lambda) + U(J)$$

The first three terms define the coupled Mooney-Rivlin matrix response. The third term is the fiber response which is a function of the fiber stretch λ and is defined as in [59]. For U, the following form is chosen in FEBio.

$$U(J) = \frac{1}{2} k (\ln J)^2$$

where $J = \det \mathbf{F}$is the Jacobian of the deformation.

Example:

```
<material id="1" type="coupled trans-iso Mooney-Rivlin">
  <c1>1</c1>
  <c2>0.1</c2>
  <c3>1</c3>
  <c4>1</c4>
  <c5>1.34</c5>
  <lam_max>1.3</lam_max>
  <k>100</k>
</material>
```

4.1.3.27 Coupled Transversely Isotropic Veronda-Westmann

This material describes a transversely isotropic Veronda-Westmann material using a fully-coupled formulation. It is define through the *coupled trans-iso Veronda-Westmann* material type. The following material parameters must be defined.

c1	Veronda-Westmann c_1 parameter.	[**P**]
c2	Veronda-Westmann c_2 parameter.	[ ]
c3	exponential multiplier	[**P**]
c4	fiber scale factor	[ ]
c5	fiber modulus in linear region	[**P**]
lam_max	maximum fiber straightening stretch	[ ]
k	bulk-like modulus	[**P**]

The strain-energy function for this constitutive model is defined by

$$W = c_1 \left(e^{c_2 (I_1 - 3)} - 1 \right) - \frac{1}{2} c_1 c_2 \left(I_2 - 3 \right) + F \left(\lambda \right) + U \left(J \right) .$$

The first two terms define the coupled Veronda-Westmann matrix response. The third term is the fiber response which is a function of the fiber stretch λ and is defined as in [59]. For U, the following form is chosen in FEBio.

$$U \left(J \right) = \frac{1}{2} k \left(\ln J \right)^2$$

where $J = \det \mathbf{F}$is the Jacobian of the deformation.

Example:

```
<material id="1" type="coupled trans-iso Veronda-Westmann">
  <c1>1</c1>
  <c2>0.1</c2>
  <c3>1</c3>
  <c4>1</c4>
  <c5>1.34</c5>
  <lam_max>1.3</lam_max>
  <k>100</k>
</material>
```

4.1.3.28 Large Poisson's Ratio Ligament

This material describes a coupled, transversely isotropic material that will conform to a particular Poisson's ratio when stretched along the fiber direction [54]. The following material parameters must be defined:

c1	Fiber coefficient c_1
c2	Fiber coefficient c_2
mu	Matrix coefficient μ
v0	Poisson's ratio parameter v_0
m	Poisson's ratio parameter m
k	Volumetric penalty coefficient κ

The strain energy function for this constitutive model is a three part expression:

$$W = W_{\text{fiber}} + W_{\text{matrix}} + W_{\text{vol}},$$

where:

$$W_{\text{fiber}} = \frac{1}{2}\frac{c_1}{c_2}\left(e^{c_2(\lambda-1)^2-1}\right),$$
$$W_{\text{matrix}} = \frac{\mu}{2}(I_1-3) - \mu\ln\left(\sqrt{I_3}\right),$$
$$W_{\text{vol}} = \frac{\kappa}{2}\left(\ln\left(\frac{I_5 - I_1 I_4 + I_2}{I_4^{2(m-v_0)}e^{-4m(\lambda-1)}}\right)\right)^2.$$

In the equations above, λ is the stretch ratio of the material along the fiber direction. The desired Poisson's ratio must first be selected based on available data for uniaxial tension along the fiber direction. The function with which to fit the Poisson's ratio data is:

$$v = -\frac{\lambda^{m-v_0}e^{-m(\lambda-1)} - 1}{\lambda - 1}.$$

The volumetric penalty coefficient κ must be selected to be large enough to enforce the Poisson's function above. If this material is to be used in a biphasic representation, κ must be selected based on experimental stress-relaxation data, since κ has an effect on the biphasic behavior of the material. Once κ, v_0, and m are chosen, c_1, c_2 and μ should be selected by fitting the stress-strain behavior of the material to experimental data. The Cauchy stress of the material is given by:

$$\boldsymbol{\sigma} = \frac{2}{J}\left((W_1 + I_1 W_2)\,\mathbf{B} - W_2\mathbf{B}^2 + W_3\,(I_3\mathbf{1}) + W_4 I_4\,(\mathbf{a}\otimes\mathbf{a}) + W_5 I_4\,(\mathbf{a}\otimes\mathbf{a}\cdot\mathbf{B} + \mathbf{B}\cdot\mathbf{a}\otimes\mathbf{a})\right)$$

where J is the jacobian of the deformation gradient $\mathbf{F}$, $\mathbf{B} = \mathbf{F}\cdot\mathbf{F}^T$ is the left Cauchy-Green deformation tensor, $\mathbf{1}$ is the 3×3 identity tensor**,** $\mathbf{a}$ is the fiber orientation vector in the deformed configuration.

Example:

```
<material id="1" name="Material1" type="PRLig">
  <c1>90</c1>
  <c2>160</c2>
  <mu>0.025</mu>
```

```
    <v0>5.85</v0>
    <m>-100</m>
    <k>1.55</k>
  </material>
```

4.2 Continuous Fiber Distribution

A continuous fiber distribution has a strain energy density that integrates the contributions from fiber bundles oriented along all directions emanating from a point in the continuum,

$$\Psi_r\left(\mathbf{C}\right) = \int_A H\left(I_n - 1\right) R\left(\mathbf{n}\right) \Psi_n\left(I_n\right)\, dA\,,$$

where $\mathbf{n}$ is the unit vector along the fiber orientation in the reference configuration, $I_n = \mathbf{n}\cdot\mathbf{C}\cdot\mathbf{n}$ is the normal component of $\mathbf{C}$ along $\mathbf{n}$ (also the square of the stretch ratio along that direction), and A represents the unit sphere (for 3D fiber distributions) or unit circle (for 2D fiber distributions) over which the integration is performed [**?**]. Thus, $\mathbf{n}$ spans all directions from the origin to points on the unit sphere or unit circle. In the integrand, Ψ_n represents the strain energy density of the fiber bundle oriented along $\mathbf{n}$; $H\left(\cdot\right)$ is the Heaviside unit step function that includes only fibers that are in tension; and $R\left(\mathbf{n}\right)$ is the fiber density distribution function that specifies the spatial fractional distribution of fibers. This function satisfies the constraint

$$\int_A R\left(\mathbf{n}\right)\, dA = 1\,.$$

For a material with an uncoupled strain energy density the corresponding expression is

$$\tilde{\Psi}_r\left(\tilde{\mathbf{C}}\right) = \int_A H\left(\tilde{I}_n - 1\right) R\left(\mathbf{n}\right) \tilde{\Psi}_n\left(\tilde{I}_n\right)\, dA\,,$$

where $\tilde{I}_n = \mathbf{n}\cdot\tilde{\mathbf{C}}\cdot\mathbf{n}$.

4.2.1 Compressible Continuous Fiber Distribution

The material type for a compressible continuous fiber distribution material is *"continuous fiber distribution"*. The following parameters must be defined:

<fibers>	Specification of the fiber material response $\Psi_n(I_n)$	
<distribution>	Specification of the fiber density distribution $R(\mathbf{n})$	
<scheme>	Numerical integration scheme	

The <fibers> tag encloses a description of the fiber constitutive relation and associated material properties, as may be selected from the list provided in Section 4.2.3. The <distribution> tag encloses a description of the fiber density distribution function, as may be selected from the list presented in Section 4.2.4. The <scheme> tag specifies the numerical integration scheme, as may be selected from the list presented in Section 4.2.5.

Example:

```
<material id="1" name="Material" type="solid mixture">
  <solid type="neo-Hookean">
    <density>1</density>
    <E>1</E>
    <v>0.3</v>
  </solid>
  <solid type="continuous fiber distribution">
    <fibers type="fiber-exponential-power-law">
      <alpha>0</alpha>
      <beta>2</beta>
      <ksi>1</ksi>
    </fibers>
    <distribution type="spherical">
    </distribution>
    <scheme type="fibers-3d-gkt">
      <nph>7</nph>
      <nth>11</nth>
    </scheme>
  </solid>
</material>
```

4.2.2 Uncoupled Continuous Fiber Distribution

The material type for an uncoupled continuous fiber distribution material is *"continuous fiber distribution uncoupled"*. The following parameters must be defined:

<fibers>	Specification of the fiber material response $\tilde{\Psi}_n\left(\tilde{I}_n\right)$
<distribution>	Specification of the fiber density distribution $R(\mathbf{n})$
<scheme>	Numerical integration scheme

The <fibers> tag encloses a description of the fiber constitutive relation and associated material properties, as may be selected from the list provided in Section 4.2.3. The <distribution> tag encloses a description of the fiber density distribution function, as may be selected from the list presented in Section 4.2.4. The <scheme> tag specifies the numerical integration scheme, as may be selected from the list presented in Section 4.2.5.

Example:

```
<material id="1" name="Material" type="uncoupled solid mixture">
  <solid type="Mooney-Rivlin">
    <density>1</density>
    <c1>1</c1>
    <c2>0.3</c2>
  </solid>
  <solid type="continuous fiber distribution uncoupled">
    <fibers type="fiber-exponential-power-law-uncoupled">
      <alpha>0</alpha>
      <beta>2</beta>
      <ksi>1</ksi>
    </fibers>
    <distribution type="spherical">
    </distribution>
    <scheme type="fibers-3d-gkt">
      <nph>7</nph>
      <nth>11</nth>
    </scheme>
  </solid>
</material>
```

4.2.3 Fibers

A fiber material is needed in the specification of a continuous fiber distribution. Use the uncoupled version of the fiber material when modeling an uncoupled continuous fiber distribution.

4.2.3.1 Fiber with Exponential-Power Law

This material type is "*fiber-exponential-power-law*". The following material parameters need to be defined:

<ksi>	ξ, representing a measure of the fiber modulus	[**P**]
<alpha>	α, coefficient of exponential argument	[ ]
<beta>	β, power of exponential argument	[ ]

The fiber strain energy density is given by

$$\Psi_n\left(I_n\right) = \frac{\xi}{\alpha\beta}\left(\exp\left[\alpha\left(I_n-1\right)^{\beta}\right]-1\right) ,$$

where $\xi > 0$, $\alpha \geqslant 0$, and $\beta \geqslant 2$.

Note: In the limit when $\alpha \to 0$, this expressions produces a power law,

$$\lim_{\alpha\to 0}\Psi_n\left(I_n\right) = \frac{\xi}{\beta}\left(I_n-1\right)^{\beta} .$$

Note: When $\beta > 2$, the fiber modulus is zero at the strain origin ($I_n = 1$). Therefore, use $\beta > 2$ when a smooth transition in the stress is desired from compression to tension.

Example:

```
<fibers type="fiber-exponential-power-law">
  <alpha>5</alpha>
  <beta>2</beta>
  <ksi>1</ksi>
</fibers>
```

4.2.3.2 Fiber with Neo-Hookean Law

This material type is "*fiber-NH*". The following material parameters need to be defined:

<mu>	μ, representing a measure of the fiber modulus	[**P**]

The fiber strain energy density is given by

$$\Psi_n\left(I_n\right) = \frac{\mu}{4}\left(I_n - 1\right)^2 \ ,$$

where $\mu > 0$.

Example:

```
<fibers type="fiber-NH">
  <mu>1</mu>
</fibers>
```

4.2.3.3 Fiber with Toe-Linear Response

This material type is "*fiber-power-linear*". The following material parameters need to be defined:

<E>	E, the fiber modulus in the linear range ($E \geqslant 0$)	[**P**]
<beta>	β, the power-law exponent in the toe region ($\beta \geqslant 2$)	[ ]
<lam0>	λ_0, the stretch ratio when the toe region transitions to the linear region ($\lambda_0 > 1$)	[ ]

The fiber strain energy density is given by

$$\Psi_n\left(I_n\right) = \begin{cases} 0 & I_n < 1 \\ \frac{\xi}{2\beta}\left(I_n - 1\right)^{\beta} & 1 \leqslant I_n \leqslant I_0 \\ E\left(I_0^{1/2} - I_n^{1/2}\right) + B\left(I_n - I_0\right) + \Psi_0 & I_0 < I_n \end{cases},$$

where $I_0 = \lambda_0^2$,

$$\xi = \frac{E}{2\left(\beta - 1\right)} I_0^{-3/2}\left(I_0 - 1\right)^{2-\beta},\ B = \frac{E I_0^{-3/2}}{2}\left[\frac{\left(I_0 - 1\right)}{2\left(\beta - 1\right)} + I_0\right],\ \Psi_0 = \frac{\xi}{2\beta}\left(I_0 - 1\right)^{\beta}$$

Example:

```
<fibers type="fiber-power-linear">
  <E>1</E>
  <beta>2.5</beta>
  <lam0>1.06</lam0>
</fibers>
```

4.2.3.4 Fiber with Exponential-Power Law Uncoupled

This material type is "*fiber-exponential-power-law-uncoupled*". The following material parameters need to be defined:

<ksi>	ξ, representing a measure of the fiber modulus	[**P**]
<alpha>	α, coefficient of exponential argument	[ ]
<beta>	β, power of exponential argument	[ ]

The fiber strain energy density is given by

$$\tilde{\Psi}_n\left(\tilde{I}_n\right) = \frac{\xi}{\alpha\beta}\left(\exp\left[\alpha\left(\tilde{I}_n - 1\right)^{\beta}\right] - 1\right),$$

where $\xi > 0$, $\alpha \geqslant 0$, and $\beta \geqslant 2$.

Note: In the limit when $\alpha \to 0$, this expressions produces a power law,

$$\lim_{\alpha\to 0} \tilde{\Psi}_n\left(\tilde{I}_n\right) = \frac{\xi}{\beta}\left(\tilde{I}_n - 1\right)^{\beta}.$$

Note: When $\beta > 2$, the fiber modulus is zero at the strain origin ($\tilde{I}_n = 1$). Therefore, use $\beta > 2$ when a smooth transition in the stress is desired from compression to tension.

Example:

```
<fibers type="fiber-exponential-power-law-uncoupled">
  <alpha>5</alpha>
  <beta>2</beta>
  <ksi>1</ksi>
</fibers>
```

4.2.3.5 Fiber with Neo-Hookean Law Uncoupled

This material type is "*fiber-NH-uncoupled*". The following material parameters need to be defined:

<mu>	μ, representing a measure of the fiber modulus	[**P**]

The fiber strain energy density is given by

$$\tilde{\Psi}_n\left(I_n\right) = \frac{\mu}{4}\left(\tilde{I}_n - 1\right)^2 ,$$

where $\mu > 0$.

Example:

```
<fibers type="fiber-NH-uncoupled">
  <mu>1</mu>
</fibers>
```

4.2.4 Distribution

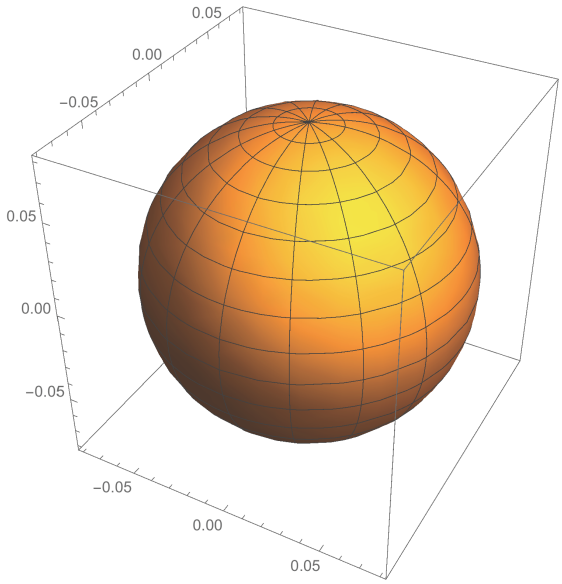
A fiber density distribution function is needed in the specification of a continuous fiber distribution.

4.2.4.1 Spherical

The fiber density distribution type "*spherical*" models an isotropic 3D distribution. This distribution corresponds to

$$R(\mathbf{n}) = \frac{1}{4\pi}.$$

It requires no additional parameters.



Example:

```
<distribution type="spherical">
</distribution>
```

4.2.4.2 Ellipsoidal

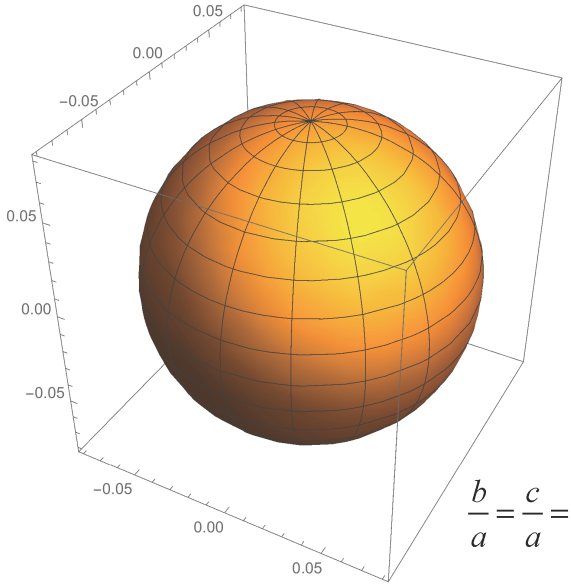
The fiber density distribution type "*ellipsoidal*" models a generally orthotropic 3D distribution. It corresponds to

$$R(\mathbf{n}) = C^{-1}\left[\left(\frac{n_1}{a}\right)^2 + \left(\frac{n_2}{b}\right)^2 + \left(\frac{n_3}{c}\right)^2\right]^{-1/2},$$

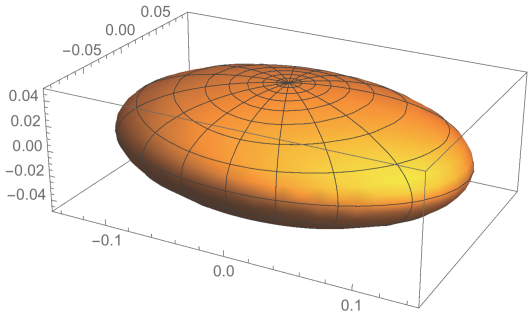
where (n_1, n_2, n_3) are the components of $\mathbf{n}$ in the local Cartesian basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ of each element, when specified (see Section 4.1.1) or the global basis by default; and C is calculated to satisfy the integration constraint on $R(\mathbf{n})$. The parameters (a, b, c) represents the semi-principal axes of the ellipsoid and must be positive. The following material parameters need to be defined:

<spa>	The semi-principal axes (a, b, c) of the ellipsoid	[ ]

The value of C is automatically adjusted to account for the values of the semi-principal axes (a, b, c). Therefore, only the relative ratios of these parameters matter.



$$\frac{b}{a} = \frac{c}{a} = 1$$



$$\frac{b}{a} = \frac{2}{3}, \frac{c}{a} = \frac{1}{3}$$

Example:

```
<distribution type="ellipsoidal">
  <spa>3,2,1</spa>
</distribution>
```

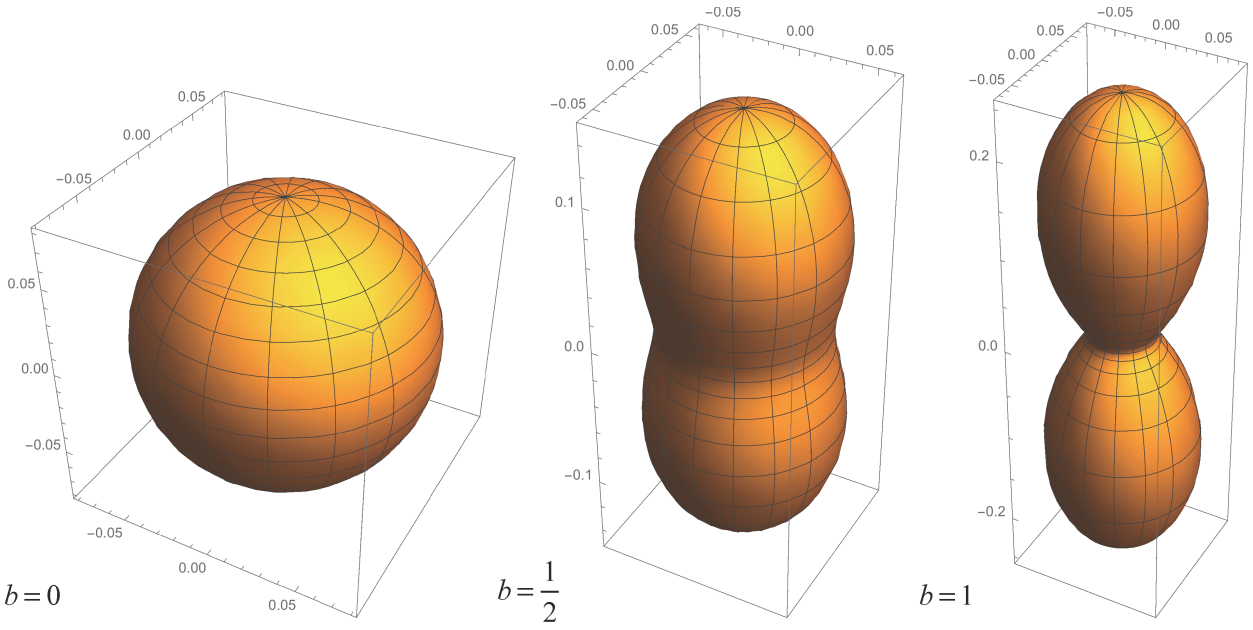
4.2.4.3 $\pi-$Periodic von Mises Distribution

The fiber density distribution type "*von-Mises-3d*" models a transversely isotropic 3D distribution [28]. It corresponds to

$$R(\mathbf{n}) = \frac{1}{\pi}\sqrt{\frac{b}{2\pi}}\frac{\exp\left(2bn_1^2\right)}{\text{erfi}\left(\sqrt{2b}\right)},$$

where (n_1, n_2, n_3) are the components of $\mathbf{n}$ in the local Cartesian basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ of each element, when specified (see Section 4.1.1) or the global basis by default; and b is the concentration parameter ($b > 0$). The following material parameters need to be defined:

<b>	The concentration parameter b	[ ]



Example:

```
<distribution type="von-Mises-3d">
  <b>0.5</b>
</distribution>
```

4.2.4.4 Circular

The fiber density distribution type "*circular*" models a transversely isotropic 2D distribution. This distribution corresponds to

$$R(\mathbf{n}) = \frac{1}{2\pi}.$$

It requires no additional parameters.

Example:

```
<distribution type="circular">
</distribution>
```

4.2.4.5 Elliptical

The fiber density distribution type "*elliptical*" models an orthotropic 2D distribution. This distribution corresponds to

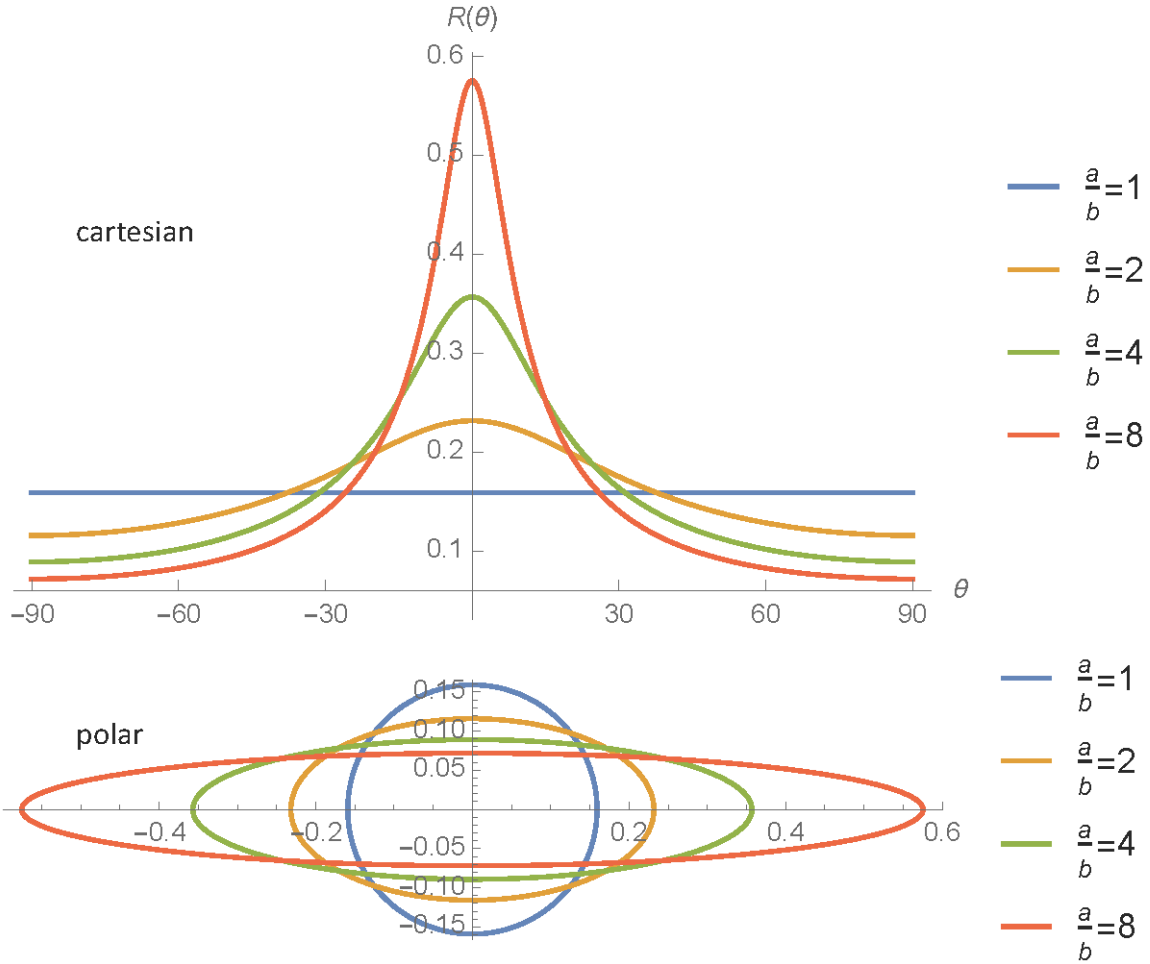
$$R(\mathbf{n}) = C^{-1}\left[\left(\frac{n_1}{a}\right)^2 + \left(\frac{n_2}{b}\right)^2\right]^{-1/2}$$

where (n_1, n_2, n_3) are the components of $\mathbf{n}$ in the local Cartesian basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ of each element, when specified (see Section 4.1.1) or the global basis by default, implying that the elliptical distribution lies in the $\{\mathbf{e}_1, \mathbf{e}_2\}$ plane; and (a, b) are the semi-principal axes of the ellipse. Here, $C = 4bK(e)$ where K is the complete elliptic integral of the first kind and

$$e = \sqrt{1 - \frac{b^2}{a^2}}$$

is the ellipse eccentricity. The following material parameters need to be defined:

<spa1>	The semi-principal axis a of the ellipse	[ ]
<spa2>	The semi-principal axis b of the ellipse	[ ]



Example:

```
<distribution type="elliptical">
  <spa1>8</spa1>
  <spa2>1</spa2>
</distribution>
```

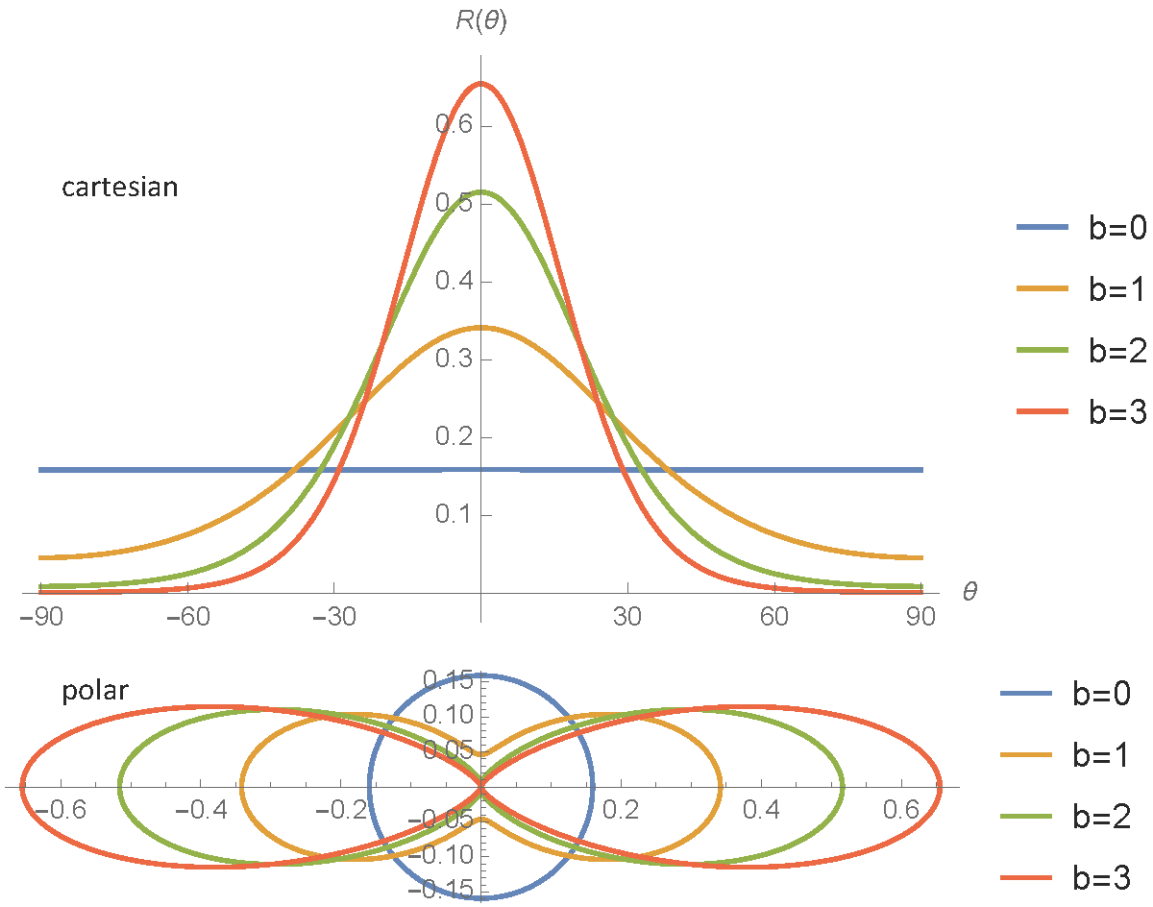
4.2.4.6 von Mises Distribution

The fiber density distribution type "*von-Mises-2d*" models an orthotropic 2D distribution. This distribution corresponds to

$$R(\mathbf{n}) = \frac{\exp\left[b\left(2n_1^2 - 1\right)\right]}{2\pi I_0(b)}$$

where (n_1, n_2, n_3) are the components of $\mathbf{n}$ in the local Cartesian basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ of each element, when specified (see Section 4.1.1) or the global basis by default, with the distribution lying in the $\{\mathbf{e}_1, \mathbf{e}_2\}$ plane; and b is the concentration parameter ($b > 0$). I_0 is the modified Bessel function of the first kind of order 0. The following material parameters need to be defined:

<b>	The concentration parameter b	[ ]



Example:

```
<distribution type="von-Mises-2d">
  <b>3</b>
</distribution>
```

4.2.5 Scheme

A numerical integration scheme is needed in the specification of a continuous fiber distribution to perform the integration over the unit sphere (3D) or the unit circle (2D). Use the uncoupled version of the scheme when modeling an uncoupled continuous fiber distribution.

4.2.5.1 Gauss-Kronrod Trapezoidal Rule

The scheme type for the Gauss-Kronrod trapezoidal rule is *"fibers-3d-gkt"* for compressible and uncoupled continuous fiber distributions. This integration rule should only be used with 3D fiber density distributions. This scheme automatically limits the range of integration to fibers that are in tension [33]. A Gauss-Kronrod quadrature rule is employed for integration across latitudes of the unit sphere. A trapezoidal rule is used for integration across longitudes. The following material parameters need to be defined:

<nph>	Number of integration points across latitudes	[ ]
<nth>	Number of integration points across longitudes	[ ]

The parameter <nph> must be one of the values 7, 11, 15, 19, 23 and 27. The parameter <nth> may be any number greater than 0. Odd values for <nth> produce more accurate results than even values. A recommended combination is nph=7 and nth=31. The total number of integration points is $N =$nph ×nth. Increasing values of N require increasing computational time.

Example:

```
<scheme type="fibers-3d-gkt">
  <nph>7</nph>
  <nth>31</nth>
</scheme>
```

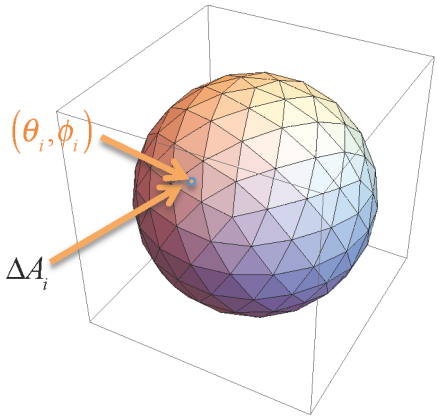
4.2.5.2 Finite Element Integration Rule

The scheme type for the finite element integration rule is *"fibers-3d-fei"* for compressible and uncoupled continuous fiber distributions. This integration rule should only be used with 3D fiber density distributions. This scheme discretizes the unit sphere into a set of N spherical triangles of nearly identical surface areas. The unit normal $\mathbf{n}$ passes through the centroid of each surface element. The integration is performed as a summation over N. For each direction $\mathbf{n}$ the stress is evaluated only if the fiber bundle is in tension along that direction. The following material parameters need to be defined:

<resolution>	the number of integration points N	[ ]

The parameter <resolution> must be one of the values 20, 34, 60, 74, 196, 210, 396, 410, 596, 610, 796, 810, 996, 1010, 1196, 1210, 1396, 1410, 1596, 1610, and 1796. A recommended combination is nph=7 and nth=31. A conservative choice for producing accurate results under general loading conditions is N =1610. Increasing values of N require increasing computational time.

$$I \approx \sum_{i=1}^{N} f\left(\theta_i, \phi_i\right) \Delta A_i$$



Example :

```
<scheme type="fibers-3d-fei">
  <resolution>1610</resolution>
</scheme>
```

4.2.5.3 Trapezoidal Rule

The scheme type for the trapezoidal integration rule is *"fibers-2d-trapezoidal"* for compressible and uncoupled continuous fiber distributions. This integration rule should only be used with 2D fiber density distributions. This scheme discretizes the unit circle into a set of N circular arcs of identical lengths. The unit normal $\mathbf{n}$ passes through the centroid of each arc element. The integration is performed as a summation over N. For each direction $\mathbf{n}$ the stress is evaluated only if the fiber bundle is in tension along that direction. The following material parameters need to be defined:

<nth>	Number of integration points N	[ ]

The parameter <nth> may be any number greater than 0. Odd values for <nth> produce more accurate results than even values.

Example:

```
<scheme type="fibers-2d-trapezoidal">
  <nth>31</nth>
</scheme>
```

4.3 Viscoelastic Solids

4.3.1 Uncoupled Viscoelastic Materials

These materials produce a viscoelastic response only for the deviatoric stress response. They must be used whenever the elastic response is uncoupled, as in the materials described in Section 4.1.2.

The material type for these materials is "uncoupled viscoelastic". The following parameters need to be defined:

<t1>-<t6>	relaxation times	**[t]**
<g1>-<g6>	viscoelastic coefficients	[ ]
<elastic>	elastic component (must be an uncoupled elastic solid)	

$$\mathbf{S}(t) = \int_{-\infty}^{t} G(t-s) \frac{d\mathbf{S}^e}{ds} ds$$

For a uncoupled viscoelastic material, the second Piola Kirchhoff stress can be written as follows [47]:

$$\mathbf{S}(t) = pJ\,\mathbf{C}^{-1} + J^{-2/3} \int_{-\infty}^{t} G(t-s) \frac{d\left(\mathrm{Dev}\left[\tilde{\mathbf{S}}^e\right]\right)}{ds} ds\,,$$

where $\tilde{\mathbf{S}}^e$ is the elastic stress derived from $\tilde{W}\left(\tilde{\mathbf{C}}\right)$ (see Section 4.1.2) and G is the relaxation function. It is assumed that the relaxation function is given by the following discrete relaxation spectrum:

$$G(t) = 1 + \sum_{i=1}^{N} \gamma_i \exp\left(-t/\tau_i\right),$$

Note that the user does not have to enter all the τ_i and γ_i coefficients. Instead, only the values that are used need to be entered. So, if N is 2, only τ_1, τ_2, γ_1 and $\gamma_2$have to be entered.

The *elastic* parameter describes the elastic material as given in Section 4.1.2.

Example:

```
<material id="1" name="Material 1" type="uncoupled viscoelastic">
  <g1>0.95</g1>
  <t1>0.01</t1>
  <elastic type="Mooney-Rivlin">
    <c1>1</c1>
    <c2>0.0</c2>
    <k>100</k>
  </elastic>
</material>
```

4.3.2 Compressible Viscoelastic Materials

The material type for viscoelastic materials is "*viscoelastic*". The following parameters need to be defined:

<t1>-<t6>	relaxation times	[**t**]
<g1>-<g6>	viscoelastic coefficients	[ ]
<elastic>	elastic component (must be a compressible elastic solid)	

For a viscoelastic material, the second Piola Kirchhoff stress can be written as follows [47]:

$$\mathbf{S}(t) = \int_{-\infty}^{t} G(t-s) \frac{d\mathbf{S}^e}{ds} ds ,$$

where $\mathbf{S}^e$ is the elastic stress and G is the relaxation function. It is assumed that the relaxation function is given by the following discrete relaxation spectrum:

$$G(t) = 1 + \sum_{i=1}^{N} \gamma_i \exp(-t/\tau_i) ,$$

Note that the user does not have to enter all the τ_i and γ_i coefficients. Instead, only the values that are used need to be entered. So, if N is 2, only τ_1, τ_2, γ_1 and $\gamma_2$have to be entered.

The *elastic* parameter describes the elastic material as given in Section 4.1.3.

Example:

```
<material id="1" name="Material 1" type="viscoelastic">
  <g1>0.95</g1>
  <t1>0.01</t1>
  <elastic type="neo-Hookean">
    <E>1</E>
    <v>0.0</v>
  </elastic>
</material>
```

4.4 Reactive Viscoelastic Solid

Reactive viscoelasticity models a material as a mixture of strong bonds, which are permanent, and weak bonds, which break and reform in response to loading [10]. Strong bonds produce the equilibrium elastic response, whereas weak bonds produce the transient viscous response. For a compressive reactive viscoelastic solid, the strain energy density is given by

$$\Psi_r\left(\mathbf{F}\right) = \Psi_r^e\left(\mathbf{F}\right) + \sum_u w^u \Psi_0^b\left(\mathbf{F}^u\right)$$

where Ψ_r^e is the strain energy density of strong bonds and Ψ_0^b is the strain energy density of weak bonds, when they all belong to the same generation. $\mathbf{F}$ is the deformation gradient of the strong bonds and the initial weak bond generation, wherease $\mathbf{F}^u$ is the relative deformation gradient for the $u-$generation weak bonds, such that $\mathbf{F}^u = \mathbf{I}$ at time u. In this expression, $w^u\left(\mathbf{X}, t\right)$ is the mass fraction of $u-$generation weak bonds, which evolves over time as described next. The summation is taken over all generations u that were created prior to the current time t.

Any number of valid solutions may exist for w^u, based on constitutive assumptions for the weak bond mass fraction supply $\hat{w}^u$. In particular, for $u-$generation bonds reforming in an unloaded state during the time interval $u \leqslant t < v$, and subsequently breaking in response to loading at $t = v$, Type I bond kinetics provides a solution of the form

$$w^u\left(\mathbf{X}, t\right) = \begin{cases} 0 & t < u \\ f^u\left(\mathbf{X}, t\right) & u \leqslant t < v \\ f^u\left(\mathbf{X}, v\right) g\left(\mathbf{F}^u\left(v\right); \mathbf{X}, t - v\right) & v \leqslant t \end{cases}$$

where

$$f^u\left(\mathbf{X}, t\right) = 1 - \sum_{\gamma < u} w^\gamma\left(\mathbf{X}, t\right)$$

and $g\left(\mathbf{F}^u\left(v\right); \mathbf{X}, t - v\right)$ is a reduced relaxation function which may assume any number of valid forms. (A reduced relaxation function $g\left(t\right)$ satisfies $g\left(0\right) = 1$ and $g\left(t \to \infty\right) = 0$, and decreases monotonically with t.) In particular, g may depend on the strain at time v relative to the reference configuration of the $u-$generation. In the recursive expression above, the earliest generation $u = -\infty$, which is initially at rest, produces $w^u\left(t\right) = 1$ for $t < v$ and $w^u\left(t\right) = g\left(\mathbf{F}^u\left(v\right); \mathbf{X}, t - v\right)$ for $t \geqslant v$; this latter expression seeds the recursion for subsequent generations. Therefore, providing a functional form for g suffices to produce the solution for all bond generations u.

For Type II bond kinetics, the solution for the mass fractions is given by

$$w^u\left(t\right) = \begin{cases} 0 & t < u \\ 1 - g\left(t - u\right) & u \leqslant t < v \\ g\left(t - v\right) - g\left(t - u\right) & v \leqslant t \end{cases} .$$

For this type of bond kinetics, the reduced relaxation function g cannot depend on the magnitude of the strain, because strain-dependence might violate the constraint $0 \leqslant w^u \leqslant 1$.

For all bond kinetics, it is also possible to constrain the occurrence of the breaking-and-reforming reaction to specific forms of the strain. For example, the reaction may be allowed to proceed only in the case of dilatational strain, or only in the case of distortional strain.

For a material with an uncoupled formulation, the strain energy density has the form

$$\Psi_r\left(\mathbf{F}\right) = U\left(J\right) + \tilde{\Psi}_r^e\left(\tilde{\mathbf{F}}\right) + \sum_u w^u \tilde{\Psi}_0^b\left(\tilde{\mathbf{F}}^u\right)$$

where $\tilde{\mathbf{F}} = J^{-1/3}\mathbf{F}$.

The material type for a compressive reactive viscoelastic solid is “reactive viscoelastic”. For the uncoupled formulation the material type is “uncoupled reactive viscoelastic”. The following parameters need to be defined:

<kinetics>	Bond kinetics type	[ ]
<trigger>	Strain invariants that trigger weak bond breakage and reformation	[ ]
<elastic>	Elastic (strong bond) material	
<bond>	Weak bond material	
<relaxation>	Reduced relaxation function	

The <kinetics> parameter should be set to 1 for Type I bond kinetics or 2 for Type II bond kinetics. The <trigger> parameter should be set 0 when weak bonds break and reform in response to any form of the strain; it should be set to 1 when the trigger is distortional strain; and it should be set to 2 when the trigger is dilatational strain. The <elastic> and <bond> materials may be selected from the list of compressible elastic materials given in Section 4.1.3 (for “reactive viscoelastic”) or from the list of uncoupled elastic materials in Section 4.1.2 (for “uncoupled reactive viscoelastic”). The <relaxation> material may be selected from the list provided in Section 4.4.1.

Example:

```
<material id="1" name="RV solid" type="reactive viscoelastic">
  <kinetics>1</kinetics>
  <trigger>0</trigger>
  <elastic type="Holmes-Mow">
    <density>1</density>
    <E>1</E>
    <v>0.3</v>
    <beta>0.5</beta>
  </elastic>
  <bond type="Holmes-Mow">
    <density>1</density>
    <E>1</E>
    <v>0.3</v>
    <beta>0.5</beta>
  </bond>
  <relaxation type="relaxation-exponential">
    <tau>4</tau>
  </relaxation>
</material>
```

4.4.1 Relaxation Functions

4.4.1.1 Exponential

The material type for this relaxation function is “relaxation-exponential”. The following material parameters need to be defined:

<tau>	Characteristic relaxation time τ	**[t]**

The reduced relaxation function for this material type is given by

$$g(t) = e^{-t/\tau}$$

4.4.1.2 Exponential Distortional

The material type for this relaxation function is “relaxation-exp-distortion”. The following material parameters need to be defined:

<tau0>	Characteristic relaxation time τ_0	**[t]**
<tau1>	Characteristic time τ_1	
<alpha>	Power exponent α	

The reduced relaxation function for this material type is given by

$$g\left(\mathbf{F}^u(v); t-v\right) = e^{-(t-v)/\tau\left[K_2^u(v)\right]}$$

where

$$\tau\left[K_2^u(v)\right] = \tau_0 + \tau_1 \cdot \left(K_2^u(v)\right)^\alpha$$

In general, $K_2 = |\mathrm{dev}\,\boldsymbol{\eta}|$ where $\boldsymbol{\eta} = \ln \mathbf{V}$ is the spatial natural (Hencky) strain tensor and $\mathbf{V}$ is the left stretch tensor. In this expression, K_2^u is the second invariant of the natural strain tensor evaluated from the relative deformation gradient $\mathbf{F}^u$. K_2^u is evaluated at the time v when weak bonds from the $u-$generation start breaking.

4.4.1.3 Fung

The material type for this relaxation function is “relaxation-Fung”. The following material parameters need to be defined:

<tau1>	Characteristic relaxation time τ_1	**[t]**
<tau2>	Characteristic time τ_2	**[t]**

The reduced relaxation function for this material type is given by

$$g(t) = \tau_2 e^{-t/\tau_2} - \tau_1 e^{-t/\tau_1} + t\left[\mathrm{Ei}\left(-\frac{t}{\tau_2}\right) - \mathrm{Ei}\left(-\frac{t}{\tau_1}\right)\right]$$

where $\mathrm{Ei}(\cdot)$ is the exponential integral function.

4.4.1.4 Park

The material type for this relaxation function is “relaxation-Park”. The following material parameters need to be defined:

<tau>	Characteristic relaxation time τ	**[t]**
<beta>	Power exponent β	[ ]

The reduced relaxation function for this material type is given by

$$g(t) = \frac{1}{1 + \left(\frac{t}{\tau}\right)^\beta}$$

4.4.1.5 Park Distortional

The material type for this relaxation function is “relaxation-Park-distortion”. The following material parameters need to be defined:

<tau0>	Characteristic relaxation time τ_0	**[t]**
<beta0>	Power exponent at zero strain β_0	[ ]
<tau1>	Characteristic relaxation time τ_1	
<beta1>	Power exponent at zero strain β_1	
<alpha>	Power exponent α	

The reduced relaxation function for this material type is given by

$$g\left(\mathbf{F}^u\left(v\right);t-v\right)=\frac{1}{1+\left(\frac{t-v}{\tau}\right)^{\beta}}$$

where

$$\tau=\tau_0+\tau_1\cdot\left(K_2^u\left(v\right)\right)^{\alpha}$$

and

$$\beta=\beta_0+\beta_1\cdot\left(K_2^u\left(v\right)\right)^{\alpha}$$

The definition of $K_2^u\left(v\right)$ is given in Section 4.4.1.2.

4.4.1.6 Power

The material type for this relaxation function is “relaxation-power”. The following material parameters need to be defined:

<tau>	Characteristic relaxation time τ	**[t]**
<beta>	Power exponent β	[ ]

The reduced relaxation function for this material type is given by

$$g\left(t\right)=\frac{1}{\left(1+\frac{t}{\tau}\right)^{\beta}}$$

4.4.1.7 Power Distortional

The material type for this relaxation function is “relaxation-power-distortion”. The following material parameters need to be defined:

<tau0>	Characteristic relaxation time τ_0	**[t]**
<beta0>	Power exponent at zero strain β_0	[ ]
<tau1>	Characteristic relaxation time τ_1	
<beta1>	Power exponent at zero strain β_1	
<alpha>	Power exponent α	

The reduced relaxation function for this material type is given by

$$g\left(\mathbf{F}^{u}\left(v\right);t-v\right)=\frac{1}{\left(1+\frac{t-v}{\tau}\right)^{\beta}}$$

where

$$\tau=\tau_{0}+\tau_{1}\cdot\left(K_{2}^{u}\left(v\right)\right)^{\alpha}$$

and

$$\beta=\beta_{0}+\beta_{1}\cdot\left(K_{2}^{u}\left(v\right)\right)^{\alpha}$$

The definition of $K_{2}^{u}\left(v\right)$ is given in Section 4.4.1.2.

4.5 Reactive Damage Mechanics

A material may accumulate damage over a single cycle or multiple cycles of loading which alters its properties. In the classical framework of damage mechanics this attenuation of the material properties is described by a single scalar damage variable D when the material is isotropic ($0 \leqslant D \leqslant 1$). For anisotropic materials however, classical frameworks require that we introduce a function of the fourth-order damage tensor $\mathcal{D}$ to account for anisotropic damage. In FEBio, we use a reactive damage mechanics framework where the elastic response is proportional to the total number of intact bonds in the material and where, at any given time in the loading history, D represents the mass fraction of bonds that have broken. In this reactive framework, it is possible to also model damage in anisotropic materials by assuming that multiple bond types exist in the material, each of which may get damaged under different circumstances. Each bond type b may be described by a distinct solid constituent within a solid mixture (see Sections 4.1.2.15 and 4.1.3.23), each having its own scalar damage variable D^b.

For a given bond type, the strain energy density $\Psi_r(D, \mathbf{F})$ of a damaged material is given by

$$\Psi_r = (1 - D)\,\Psi_0\,,$$

where $\Psi_0(\mathbf{F})$ is the strain energy density when all bonds of that type are intact. Here, $1 - D$ represents the mass fraction of bonds that remains intact. Similarly, the Cauchy stress $\boldsymbol{\sigma}(D, \mathbf{F})$ of the damaged material is given by

$$\boldsymbol{\sigma} = (1 - D)\,\boldsymbol{\sigma}_0\,,$$

where $\boldsymbol{\sigma}_0(\mathbf{F})$ is the stress in the intact material, at a given strain, as derived from $\Psi_0(\mathbf{F})$. The intact material may be based on any of the elastic materials described in Sections 4.1.2 and 4.1.3.

The evolution of the damage variable D is determined by a user-selected scalar damage criterion measure $\Xi(\mathbf{F})$ (Ξ is the capital form of ξ). For example, $\Xi(\mathbf{F})$ may represent the strain energy density, or von Mises stress, or maximum principal normal strain, etc. If $\Xi(\mathbf{F})$ exceeds a given threshold at some state of deformation $\mathbf{F}$, then damage may initiate or progress further. If all bonds fail at a single threshold value Ξ_m, the material undergoes fracture. More commonly, bonds may fail with increasing probability as Ξ increases over a given range. Consequently, the evolution of damage may be based on a user-selected cumulative distribution function (c.d.f.) $F(\Xi)$, such that $D(t) = F(\Xi_m)$ where Ξ_m is the maximum value of Ξ achieved over the loading history up until the current time t.

4.5.1 General Specification of Damage Materials

The material types for damage materials are *"elastic damage"* and *"uncoupled elastic damage"*. The following parameters must be defined:

<elastic>	Specification of the elastic material
<damage>	Specification of the cumulative distribution function $F(\Xi)$
<criterion>	Specification of the damage criterion Ξ

The <elastic> tag encloses a description of the constitutive relation of the intact elastic material and associated material properties, as may be selected from the list provided in Section 4.1.3 for compressible materials (used with *"elastic damage"*) and Section 4.1.2 for uncoupled materials (used with *"uncoupled elastic damage"*). The <damage> tag encloses a description of the cumulative distribution function and associated material properties, as may be selected from the list presented in Section 4.5.2. The <criterion> tag encloses a description of the damage criterion, as may be selected from the list presented in Section 4.5.3.

Example:

```
<material id="1" type="elastic damage">
  <elastic type="neo-Hookean">
    <density>1</density>
    <E>0.13</E>
    <v>0.3</v>
  </elastic>
  <damage type="CDF Weibull">
    <alpha>8</alpha>
    <mu>0.3</mu>
    <Dmax>1</Dmax>
  </damage>
  <criterion type="DC max normal Lagrange strain">
  </criterion>
</material>
```

4.5.2 Cumulative Distribution Functions

Cumulative distribution functions provide the function $F(\Xi)$ that determines the evolution of the damage variable D based on the maximum value of the failure criterion Ξ up until the current time.

4.5.2.1 Simo

The material type for Simo's c.d.f. [49] is "*CDF Simo*". The following material parameters must be defined:

<a>	Parameter α (same units as Ξ, $\alpha > 0$)	[Ξ]
<b>	Parameter β ($0 \leqslant \beta \leqslant 1$)	[ ]

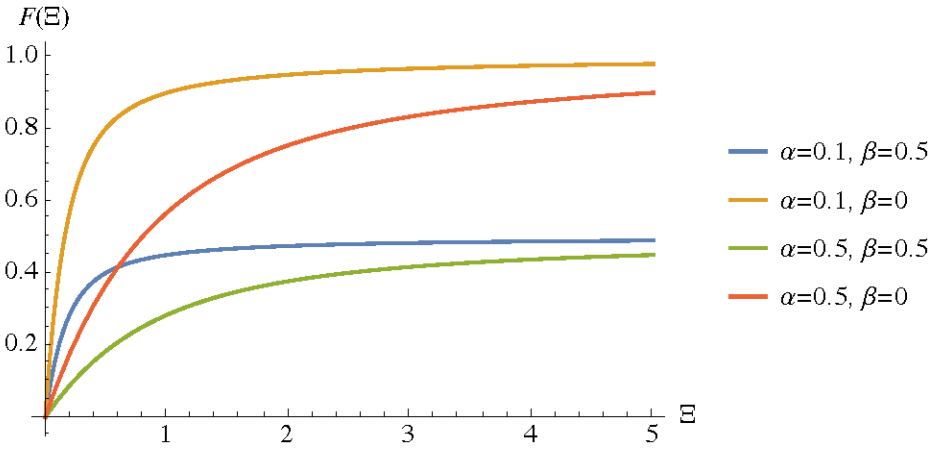
For this material the c.d.f. is given by

$$F(\Xi) = 1 - \beta - (1 - \beta)\frac{\alpha}{\Xi}\left(1 - e^{-\Xi/\alpha}\right) .$$

Note that

$$\lim_{\Xi \to \infty} F(\Xi) = 1 - \beta$$

represents the maximum allowable damage. Therefore, β regulates the maximum allowable damage, whereas α controls the rate at which $F(\Xi)$ increases with increasing Ξ.



Example:

```
<damage type="CDF Simo">
  <a>0.1</a>
  <b>0</b>
  <Dmax>1</Dmax>
</damage>
```

4.5.2.2 Log-Normal

The material type for a log-normal c.d.f. is "*CDF log-normal*". The following material parameters must be defined:

<mu>	Parameter μ (same units as Ξ, $\mu > 0$)	[Ξ]
<sigma>	Parameter σ ($\sigma > 0$)	[ ]
<Dmax>	Maximum allowable damage (optional, default is 1)	[ ]

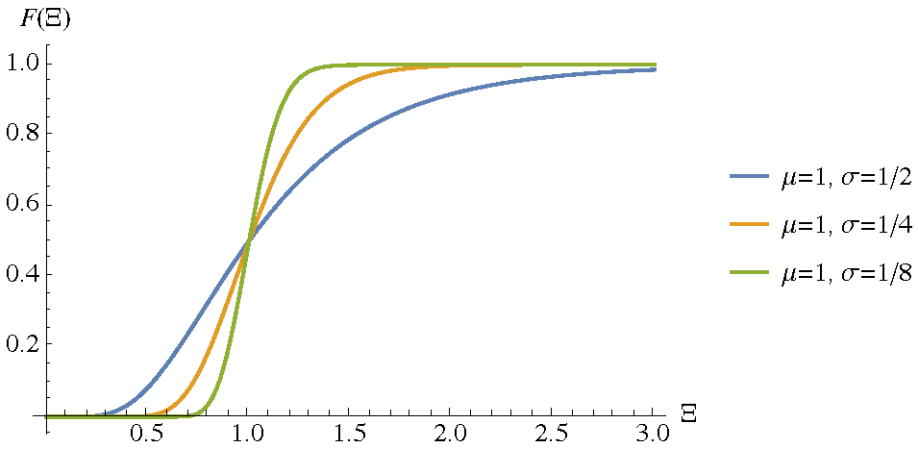
For this material the c.d.f. is given by

$$F(\Xi) = \frac{1}{2}\text{erfc}\left[-\frac{\ln(\Xi/\mu)}{\sigma\sqrt{2}}\right].$$

Note that

$$F(\mu) = 1/2,$$

which shows that μ is the value of Ξ at which half of the bonds break. Here, σ regulates the rate at which damage increases with increasing Ξ, with smaller values of σ producing a more rapid increase.



Example:

```
<damage type="CDF log-normal">
  <mu>1</mu>
  <sigma>0.5</sigma>
  <Dmax>1</Dmax>
</damage>
```

4.5.2.3 Weibull

The material type for a Weibull c.d.f. is "*CDF Weibull*". The following material parameters must be defined:

<mu>	Parameter μ (same units as Ξ, $\mu > 0$)	[Ξ]
<alpha>	Parameter α ($\alpha > 0$)	[ ]
<Dmax>	Maximum allowable damage (optional, default is 1)	[ ]

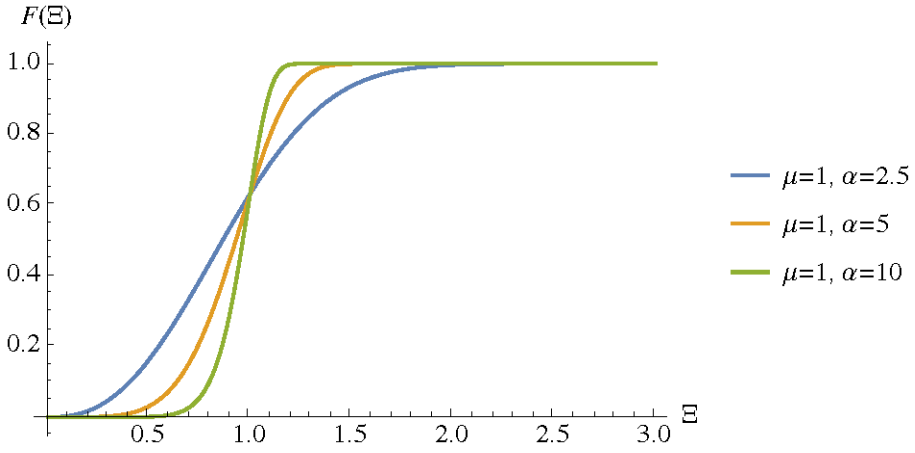
For this material the c.d.f. is given by

$$F(\Xi) = 1 - \exp\left[-(\Xi/\mu)^{\alpha}\right] .$$

Note that

$$F(\mu) = 1 - e^{-1} \approx 0.63 ,$$

which shows that μ is the value of Ξ at which the fraction $1 - e^{-1}$ of bonds break. Here, α regulates the rate at which damage increases with increasing Ξ, with higher values of α producing a more rapid increase.



Example:

```
<damage type="CDF Weibull">
  <mu>1</mu>
  <alpha>5.0</alpha>
  <Dmax>1</Dmax>
</damage>
```

4.5.2.4 Quintic Polynomial

The material type for a quintic polynomial c.d.f. is "*CDF quintic*". The following material parameters must be defined:

<mumin>	Parameter $\mu_{\min}$ (same units as Ξ, $\mu_{\min} > 0$)	[Ξ]
<mumax>	Parameter $\mu_{\max}$ (same units as Ξ, $\mu_{\max} > \mu_{\min}$)	[ ]
<Dmax>	Maximum allowable damage (optional, default is 1)	[ ]

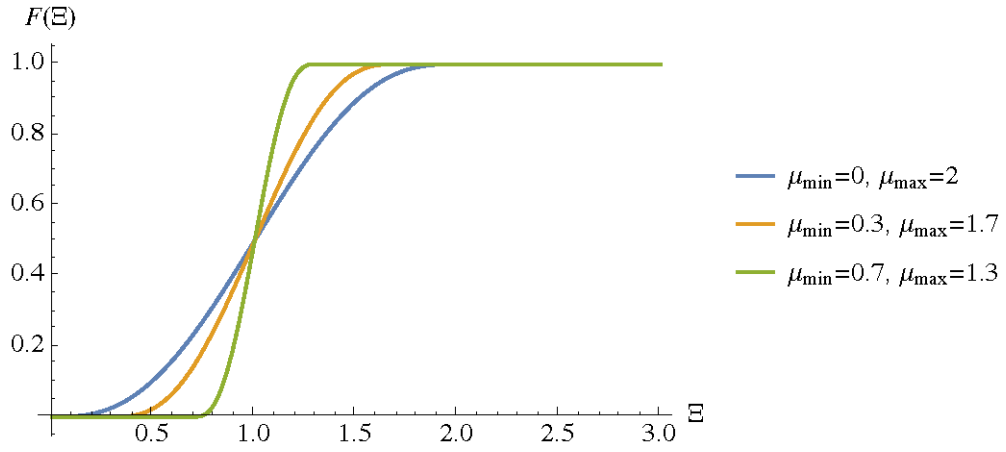
For this material the c.d.f. is given by

$$F(\Xi) = \begin{cases} 0 & \Xi \leqslant \mu_{\min} \\ x^3\left(10 - 15x + 6x^2\right) & \mu_{\min} < \Xi \leqslant \mu_{\max} \\ 1 & \mu_{\max} < \Xi \end{cases}, \quad x = \frac{\Xi - \mu_{\min}}{\mu_{\max} - \mu_{\min}}.$$

Note that

$$F\left(\frac{1}{2}\left(\mu_{\min} + \mu_{\max}\right)\right) = \frac{1}{2},$$

which shows that $\left(\mu_{\min} + \mu_{\max}\right)/2$ is the value of Ξ at which half of the bonds break. The range $\mu_{\max} - \mu_{\min}$ regulates the rate at which damage increases with increasing Ξ, with a narrower range producing a more rapid increase.



Example:

```
<damage type="CDF quintic">
  <mumin>0.3</mumin>
  <mumax>1.7</mumax>
  <Dmax>1</Dmax>
</damage>
```

4.5.2.5 Step

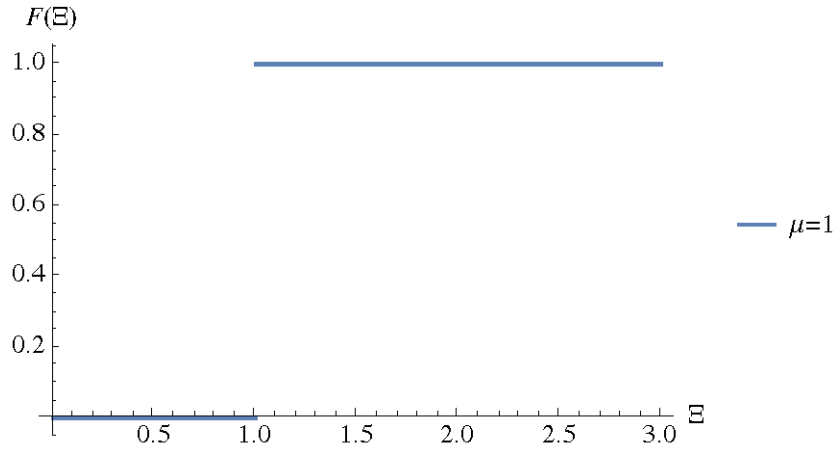
The material type for a step c.d.f. is "*CDF step*". The following material parameters must be defined:

<mu>	Parameter μ (same units as Ξ)	[Ξ]
<Dmax>	Maximum allowable damage (optional, default is 1)	[ ]

For this material the c.d.f. is given by

$$F(\Xi) = H(\Xi) \quad ,$$

where $H(\cdot)$ is the Heaviside unit step function. The step c.d.f. may be used to model fracture.



Example:

```
<damage type="CDF step">
  <mu>1.0</mu>
  <Dmax>1</Dmax>
</damage>
```

4.5.3 Damage Criterion

The damage criterion provides the functional form of $\Xi(\mathbf{F})$ that determines the evolution of damage. There are no material parameters associated with these functions. All the functions currently modeled in FEBio are defined over the range $\Xi \in [0, \infty[$.

4.5.3.1 Simo

The material type for Simo's damage criterion [49] is "*DC Simo"*. For this criterion,

$$\Xi(\mathbf{F}) = \sqrt{2\Psi_0(\mathbf{F})}$$

Example:

```
<criterion type="DC Simo"/>
```

4.5.3.2 Strain Energy Density

The material type for strain energy density damage criterion is "*DC strain energy density"*. For this criterion,

$$\Xi(\mathbf{F}) = \Psi_0(\mathbf{F})$$

Example:

```
<criterion type="DC strain energy density"/>
```

4.5.3.3 Specific Strain Energy

The material type for specific strain energy damage criterion is *"DC specific strain energy"*. For this criterion,

$$\Xi(\mathbf{F}) = \Psi_0(\mathbf{F})/\rho$$

where ρ is the elastic material's density.

Example:

```
<criterion type="DC specific strain energy"/>
```

4.5.3.4 Von Mises Stress

The material type for von Mises stress damage criterion is *"DC von Mises stress"*. For this criterion,

$$\Xi(\mathbf{F}) = \sqrt{\frac{1}{2}\left[(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2\right]}$$

where $\sigma_1, \sigma_2, \sigma_3$ are the principal values of $\boldsymbol{\sigma}_0(\mathbf{F})$.

Example:

```
<criterion type="DC von Mises stress"/>
```

4.5.3.5 Maximum Shear Stress

The material type for maximum shear stress damage criterion is *"DC max shear stress"*. For this criterion,

$$\Xi\left(\mathbf{F}\right)=\max\left(\frac{\left|\sigma_1-\sigma_2\right|}{2},\frac{\left|\sigma_2-\sigma_3\right|}{2},\frac{\left|\sigma_3-\sigma_1\right|}{2}\right)$$

where $\sigma_1,\sigma_2,\sigma_3$ are the principal values of $\boldsymbol{\sigma}_0\left(\mathbf{F}\right)$.

Example:

```
<criterion type="DC max shear stress"/>
```

4.5.3.6 Maximum Normal Stress

The material type for maximum normal stress damage criterion is *"DC max normal stress"*. For this criterion,

$$\Xi\left(\mathbf{F}\right)=\max\left(\sigma_1,\sigma_2,\sigma_3\right)$$

where $\sigma_1,\sigma_2,\sigma_3$ are the principal values of $\boldsymbol{\sigma}_0\left(\mathbf{F}\right)$.

Example:

```
<criterion type="DC max normal stress"/>
```

4.5.3.7 Maximum Normal Lagrange Strain

The material type for maximum normal Lagrange strain damage criterion is *"DC max normal Lagrange strain"*. For this criterion,

$$\Xi\left(\mathbf{F}\right)=\max\left(E_1,E_2,E_3\right)$$

where E_1,E_2,E_3 are the principal values of $\mathbf{E}=\left(\mathbf{F}^T\cdot\mathbf{F}-\mathbf{I}\right)/2$.

Example:

```
<criterion type="DC max normal Lagrange strain"/>
```

4.6 Multigeneration Solids

This type of material [6] implements a mechanism for multigenerational interstitial growth of solids whereby each growth generation γ has a distinct reference configuration $\mathbf{X}^\gamma$ determined at the time t^γ of its deposition. Therefore, the solid matrix of a growing material consists of a multiplicity of intermingled porous bodies, each representing a generation γ, all of which are constrained to move together in the current configuration $\mathbf{x}$. The deformation gradient of each generation is $\mathbf{F}^\gamma = \partial\mathbf{x}/\partial\mathbf{X}^\gamma$. The first generation ($\gamma = 1$) is assumed to be present at time $t^1 = 0$, therefore its reference configuration is $\mathbf{X}^1 \equiv \mathbf{X}$ and its deformation gradient $\mathbf{F}^1 = \partial\mathbf{x}/\partial\mathbf{X}^1$ is equivalent to $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$. Each generation's reference configuration $\mathbf{X}^\gamma$ has a one-to-one mapping $\mathbf{F}^{\gamma 1} = \partial\mathbf{X}^\gamma/\partial\mathbf{X}^1$ with the master reference configuration $\mathbf{X}^1$, which is that of the first generation. This mapping is postulated based on a constitutive assumption with regard to that generation's state of stress at the time of its deposition. In the current implementation, the newly deposited generation is assumed to be in a stress-free state, even though the underlying material is in a loaded configuration. Therefore, the mapping between generation γ and the first generation is simply $\mathbf{F}^{\gamma 1} = \mathbf{F}^1\left(\mathbf{X}^1, t^\gamma\right) \equiv \mathbf{F}\left(\mathbf{X}, t^\gamma\right)$. In other words, when generation γ first comes into existence, its reference configuration is the current configuration at time t^γ. Note that $\mathbf{F}^{\gamma 1}$ is a time-invariant (though not necessarily homogeneous) quantity that is determined uniquely at the birth of a generation.

The state of stress in a multigeneration solid is given by

$$\boldsymbol{\sigma} = \sum_\gamma \frac{1}{J^{\gamma 1}} \boldsymbol{\sigma}^\gamma\left(\mathbf{F}^\gamma\right)$$

where $\boldsymbol{\sigma}^\gamma\left(\mathbf{F}^\gamma\right)$ is the state of stress in the generation γ, as would be evaluated from a strain energy density function whose reference configuration is $\mathbf{X}^\gamma$. In the above equation, $J^{\gamma 1} = \det \mathbf{F}^{\gamma 1}$ and the factor $1/J^{\gamma 1}$ ensures that the strain energy density of each generation is properly normalized the volume of the material in the master reference configuration $\mathbf{X}^1$, when summing up the stresses in all the generations.

Multigeneration solids typically exhibit residual stresses when $\mathbf{F}^{\gamma 1}$ is inhomogeneous.

4.6.1 General Specification of Multigeneration Solids

The material type for a multigeneration solid is *"multigeneration"*[2]. This material describes a mixture of elastic solids, each created in a specific generation. It is a container for any combination of the elastic materials described.

<generation>	Definition of a generation.

The <generation> tag defines a new generation. It takes the following child elements.

<start_time>	"birth"-time for this generation	**[t]**
<solid>	Specification of the constitutive model for this generation	

The *solid* element defins the solid matrix constitutive relation and associated material properties.

Example:

[2] As of FEBio version 2.0, the format for defininig multi-generation materials has changed. The previous format where the generations are defined in the *Globals* section is no longer supported.

```
<material id="1" name="Growing Solid" type="multigeneration">
  <generation id="1">
    <start_time>0.0</start_time>
    <solid type="Holmes-Mow">
      <density>1</density>
      <E>1</E>
      <v>0</v>
      <beta>0.1</beta>
    </solid>
  </generation>
  <generation id="2">
    <start_time>1.0</start_time>
    <solid type="Holmes-Mow">
      <density>1</density>
      <E>1</E>
      <v>0</v>
      <beta>0.1</beta>
    </solid>
  </generation>
</material>
```

The corresponding value of t^γ for each of the generations is provided in the <Globals> section.

Example:

```
<Globals>
  <Generations>
    <gen id="1">0.0</gen>
    <gen id="2">1.0</gen>
  </Generations>
</Globals>
```

4.7 Biphasic Materials

Biphasic materials may be used to model a porous medium consisting of a mixture of a porous-permeable solid matrix and an interstitial fluid. Each of these mixture constituents is assumed to be intrinsically incompressible. This means that the true densities of the solid and fluid are invariant in space and time; this assumption further implies that a biphasic mixture will undergo zero volume change when subjected to a hydrostatic fluid pressure. Yet the mixture is compressible because the pores of the solid matrix may gain or lose fluid under general loading conditions. The Cauchy stress $\boldsymbol{\sigma}$ in a biphasic material is given by

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}^e \,, \tag{4.7.1}$$

where p is the interstitial fluid pressure and $\boldsymbol{\sigma}^e$ is the stress resulting from the deformation of the porous solid matrix. Therefore, the constitutive relation of the solid matrix should be chosen from the list of compressible materials provided in Section 4.1.3. The user is referred to the *FEBio Theory Manual* for a general description of the biphasic theory.

In addition to selecting a constitutive relation for the solid matrix, a constitutive relation must also be selected for the hydraulic permeability of the interstitial fluid flowing within the porous deformable solid matrix. The hydraulic permeability relates the volumetric flux of the fluid relative to the solid, $\mathbf{w}$, to the interstitial fluid pressure gradient, ∇p, according to

$$\mathbf{w} = -\mathbf{k} \cdot \operatorname{grad} p \,, \tag{4.7.2}$$

where $\mathbf{k}$ is the hydraulic permeability tensor. (Note that this expression does not account for the contribution of external body forces on the fluid.)

The governing equations for biphasic materials are the mixture momentum balance under quasi-static conditions, in the absence of external body force,

$$\operatorname{div} \boldsymbol{\sigma} = -\operatorname{grad} p + \operatorname{div} \boldsymbol{\sigma}^e = \mathbf{0} \,, \tag{4.7.3}$$

and the mixture mass balance,

$$\operatorname{div} (\mathbf{v}^s + \mathbf{w}) = 0 \,, \tag{4.7.4}$$

where $\mathbf{v}^s$ is the solid velocity.

4.7.1 General Specification of Biphasic Materials

The material type for a biphasic material is *"biphasic"*. The following parameters must be defined:

<solid>	Specification of the solid matrix	
<phi0>	solid volume fraction φ_r^s in the reference configuration $(0 < \varphi_r^s < 1)$	[ ]
<fluid_density>	Fluid density ρ_T^w	
<permeability>	Specification of the hydraulic permeability	
<solvent_supply>	Specification of the fluid supply $\hat{\varphi}^w$	

The <solid> tag encloses a description of the solid matrix constitutive relation and associated material properties, as may be selected from the list provided in Section 4.1.3. The <permeability> tag encloses a description of the permeability constitutive relation and associated material properties, as may be selected from the list presented in Section 4.7.2. The parameter <phi0> must be greater than 0 (no solid) and less than 1 (no porosity). The volume fraction of fluid (also known as the porosity) in the reference configuration is given by $1 - \varphi_r^s$. The fluid density ρ_T^w specified in <fluid_density> and the solid density ρ_T^s specified in <density> within the <solid> tag are needed only when body forces are prescribed.

Example:

```
<material id="1" name="Biphasic tissue" type="biphasic">
  <solid name="Elasticity" type="neo-Hookean">
    <E>1.0</E>
    <v>0.3</v>
  </solid>
  <phi0>0.2</phi0>
  <permeability name="Permeability" type="perm-const-iso">
    ... (description of permeability material)
  </permeability>
</material>
```

4.7.2 Permeability Materials

Permeability materials provide a constitutive relation for the hydraulic permeability of a biphasic material.

4.7.2.1 Constant Isotropic Permeability

The material type for constant isotropic permeability is "*perm-const-iso"*. The following material parameters must be defined:

<perm>	hydraulic permeability k	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]

This isotropic material model uses the biphasic theory for describing the time-dependent material behavior of materials that consist of both a solid and fluid phase [44].

When the permeability is isotropic,

$$\mathbf{k} = k\,\mathbf{I}$$

For this material model, k is constant. Generally, this assumption is only reasonable when strains are small.

Example:

```
<permeability name="Permeability" type="perm-const-iso ">
  <perm>0.001</perm>
</permeability>
```

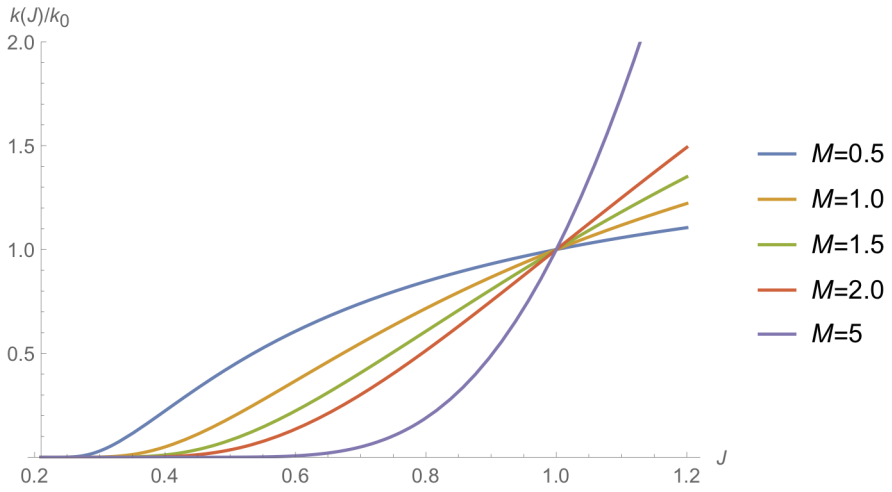


Figure 4.7.1: Exponential isotropic permeability, showing dependence of $k\left(J\right)/k_0$ on material parameter M, when $\varphi_0 = 0.2$ and $\varphi_0 < J \leq 1.2$.

4.7.2.2 Exponential Isotropic Permeability

The material type for exponential isotropic permeability is "*perm-exp-iso*". The following material parameters must be defined:

<perm>	isotropic hydraulic permeability k_0 in the reference state	[**L**^{4}/**F**·**t**]
<M>	exponential strain-dependence coefficient M ($M \geq 0$)	[ ]

This isotropic material model has the general form

$$\mathbf{k} = k\left(J\right)\,\mathbf{I}$$

where $J = \det \mathbf{F}$ is the determinant of the deformation gradient. For this material model,

$$k\left(J\right) = k_0 \exp\left(M\frac{J-1}{J-\varphi_0}\right)\,,$$

where φ_0 is the referential solid volume fraction of the porous solid matrix. Pore closure occurs as J approaches φ_0 from above, in which case the permeability reduces to zero,

$$\lim_{J\to\varphi_0} k\left(J\right) = 0\,.$$

Representative variations of $k\left(J\right)/k_0$ are shown in Figure 4.7.1.

Example:

```
<permeability name="Permeability" type="perm-exp-iso ">
  <perm>0.001</perm>
  <M>1.5</M>
</permeability>
```

4.7.2.3 Holmes-Mow

The material type for Holmes-Mow permeability is *"perm-Holmes-Mow"*. The following material parameters need to be defined:

<perm>	isotropic hydraulic permeability k_0 in the reference state	[**L**^{4}/**F**·**t**]
<M>	exponential strain-dependence coefficient M ($M \geq 0$)	[ ]
<alpha>	power-law exponent α ($\alpha \geq 0$)	[ ]

This isotropic material is similar to the constant isotropic permeability material described above, except that it uses a strain-dependent permeability tensor [32]:

$$\mathbf{k} = k\left(J\right)\mathbf{I},$$

where,

$$k\left(J\right) = k_0\left(\frac{J-\varphi_0}{1-\varphi_0}\right)^{\alpha} e^{\frac{1}{2}M\left(J^2-1\right)},$$

and J is the Jacobian of the deformation, i.e. $J = \det \mathbf{F}$ where $\mathbf{F}$ is the deformation gradient.

Example:

This example defines a permeability material of the Holmes-Mow type.

```
<permeability type="perm-Holmes-Mow">
  <perm>0.001</perm>
  <M>1.5</M>
  <alpha>2</alpha>
</permeability>
```

4.7.2.4 Referentially Isotropic Permeability

The material type for a biphasic material with strain-dependent permeability which is isotropic in the reference configuration is *"perm-ref-iso"*. The following material parameters need to be defined:

<perm0>	hydraulic permeability k_{0r}	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm1>	hydraulic permeability k_{1r}	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm2>	hydraulic permeability k_{2r}	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<M>	exponential strain-dependence coefficient M ($M \geqslant 0$)	[ ]
<alpha>	power-law exponent α ($\alpha \geqslant 0$)	[ ]

This material uses a strain-dependent permeability tensor that accommodates strain-induced anisotropy:

$$\mathbf{k} = \left(k_{0r}\mathbf{I} + \frac{k_{1r}}{J^2}\mathbf{b} + \frac{k_{2r}}{J^4}\mathbf{b}^2\right)\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha} e^{M\left(J^2-1\right)/2},$$

where J is the Jacobian of the deformation, i.e. $J = \det\mathbf{F}$ where $\mathbf{F}$ is the deformation gradient, and $\mathbf{b} = \mathbf{F}\cdot\mathbf{F}^T$ is the left Cauchy-Green tensor. Note that the permeability in the reference state ($\mathbf{F} = \mathbf{I}$) is isotropic and given by $\mathbf{k} = \left(k_{0r} + k_{1r} + k_{2r}\right)\mathbf{I}$.

Example:

```
<permeability name="Permeability" type="perm-ref-iso">
  <perm0>0.001</perm0>
  <perm1>0.005</perm1>
  <perm2>0.002</perm2>
  <M>1.5</M>
  <alpha>2</alpha>
</permeability>
```

4.7.2.5 Referentially Orthotropic Permeability

The material type for a poroelastic material with strain-dependent permeability which is orthotropic in the reference configuration is *"perm-ref-ortho"*. The following material parameters need to be defined:

<perm0>	isotropic hydraulic permeability k_{0r}	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm1>	hydraulic permeabilities k_{1r}^a along orthogonal directions ($a = 1, 2, 3$)	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm2>	hydraulic permeabilities k_{2r}^a along orthogonal directions ($a = 1, 2, 3$)	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<M0>	isotropic exponential strain-dependence coefficient M_0 ($M_0 \geqslant 0$)	[ ]
<M>	orthotropic exponential strain-dependence coefficient M_a ($a = 1, 2, 3$, $M_a \geqslant 0$)	[ ]
<alpha0>	isotropic power-law exponent α_0 ($\alpha_0 \geqslant 0$)	[ ]
<alpha>	power-law exponent α_a ($a = 1, 2, 3$, $\alpha_a \geqslant 0$)	[ ]

This material uses a strain-dependent permeability tensor that accommodates strain-induced anisotropy:

$$\mathbf{k} = k_0\mathbf{I} + \sum_{a=1}^{3} k_1^a \mathbf{m}_a + k_2^a \left(\mathbf{m}_a \cdot \mathbf{b} + \mathbf{b} \cdot \mathbf{m}_a\right) ,$$

where,

$$\begin{aligned} k_0 &= k_{0r}\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_0} e^{M_0\left(J^2-1\right)/2} \\ k_1^a &= \frac{k_{1r}^a}{J^2}\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_a} e^{M_a\left(J^2-1\right)/2}, \quad a = 1, 2, 3\,. \\ k_2^a &= \frac{k_{2r}^a}{2J^4}\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_a} e^{M_a\left(J^2-1\right)/2} \end{aligned}$$

J is the Jacobian of the deformation, i.e. $J = \det \mathbf{F}$ where $\mathbf{F}$ is the deformation gradient. $\mathbf{m}_a$ are second order tensors representing the spatial structural tensors describing the orthogonal planes of symmetry, given by

$$\mathbf{m}_a = \mathbf{F} \cdot (\mathbf{V}_a \otimes \mathbf{V}_a) \cdot \mathbf{F}^T, \quad a = 1 - 3,$$

where $\mathbf{V}_a$ are orthonormal vectors normal to the planes of symmetry (defined as described in Section 4.1.1.2). Note that the permeability in the reference state ($\mathbf{F} = \mathbf{I}$) is given by $\mathbf{k} = k_{0r}\mathbf{I} + \sum_{a=1}^{3} \left(k_{1r}^a + k_{2r}^a\right) \mathbf{V}_a \otimes \mathbf{V}_a$.

Example:

```
<permeability name="Permeability" type="perm-ref-ortho">
  <perm0>0.001</perm0>
  <perm1>0.01, 0.02, 0.03</perm1>
  <perm2>0.001, 0.002, 0.003</perm2>
  <M0>0.5</M0>
  <M>1.5, 2.0, 2.5</M>
  <alpha0>1.5</alpha0>
```

```
    <alpha>2, 2.5, 3</alpha>
</permeability>
```

4.7.2.6 Referentially Transversely Isotropic Permeability

The material type for a biphasic material with strain-dependent permeability which is transversely isotropic in the reference configuration is *"perm-ref-trans-iso"*. The following material parameters need to be defined:

<perm0>	isotropic hydraulic permeability k_{0r}	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm1A>	axial hydraulic permeability k_{1r}^A	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm2A>	axial hydraulic permeability k_{2r}^A	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm1T>	transverse hydraulic permeability k_{1r}^T	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<perm2T>	transverse hydraulic permeability k_{2r}^T	[$\mathbf{L}^4/\mathbf{F}\cdot\mathbf{t}$]
<M0>	isotropic exponential strain-dependence coefficient M_0 ($M_0 \geqslant 0$)	[ ]
<MA>	axial exponential strain-dependence coefficient M_A ($M_A \geqslant 0$)	[ ]
<MT>	transverse exponential strain-dependence coefficient M_T ($M_T \geqslant 0$)	[ ]
<alpha0>	isotropic power-law exponent α_0 ($\alpha_0 \geqslant 0$)	[ ]
<alphaA>	axial power-law exponent α_A ($\alpha_A \geqslant 0$)	[ ]
<alphaT>	transverse power-law exponent α_T ($\alpha_T \geqslant 0$)	[ ]

This material uses a strain-dependent permeability tensor that accommodates strain-induced anisotropy:

$$\begin{aligned}\mathbf{k} = {} & k_{0r}\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_0} e^{M_0\left(J^2-1\right)/2}\mathbf{I} \\ & + \left(\frac{k_{1r}^T}{J^2}\left(\mathbf{b}-\mathbf{m}\right) + \frac{k_{2r}^T}{2J^4}\left[2\mathbf{b}^2 - \left(\mathbf{m}\cdot\mathbf{b}+\mathbf{b}\cdot\mathbf{m}\right)\right]\right)\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_T} e^{M_T\left(J^2-1\right)/2}, \\ & + \left(\frac{1}{J^2}k_{1r}^A\mathbf{m} + \frac{1}{2J^4}k_{2r}^A\left(\mathbf{m}\cdot\mathbf{b}+\mathbf{b}\cdot\mathbf{m}\right)\right)\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_A} e^{M_A\left(J^2-1\right)/2}\end{aligned}$$

where J is the Jacobian of the deformation, i.e. $J = \det\mathbf{F}$ where $\mathbf{F}$ is the deformation gradient, and $\mathbf{b} = \mathbf{F}\cdot\mathbf{F}^T$ is the left Cauchy-Green tensor. $\mathbf{m}$ is a second order tensor representing the spatial structural tensor describing the axial direction, given by

$$\mathbf{m} = \mathbf{F}\cdot\left(\mathbf{V}\otimes\mathbf{V}\right)\cdot\mathbf{F}^T,$$

where $\mathbf{V}$ is a unit vector along the axial direction (defined as described in Section 4.1.1). Note that the permeability in the reference state ($\mathbf{F}=\mathbf{I}$) is given by $\mathbf{k} = \left(k_{0r}+k_{1r}^T+k_{2r}^T\right)\mathbf{I} + \left(k_{1r}^A - k_{1r}^T + k_{2r}^A - k_{2r}^T\right)\left(\mathbf{V}\otimes\mathbf{V}\right)$.

Example:

```
<permeability name="Permeability" type="perm-ref-trans-iso">
  <perm0>0.002</perm0>
  <perm1A>0.01</perm1A>
  <perm2A>0.01</perm2A>
  <perm1T>0.001</perm1T>
  <perm2T>0.05</perm2T>
  <M0>1.0</M0>
  <MA>0.5</MA>
  <MT>1.5</MT>
  <alpha0>1.0</alpha0>
  <alphaA>0.5</alphaA>
  <alphaT>2.0</alphaT>
</permeability>
```

4.7.3 Fluid Supply Materials

Fluid supply materials may be used to simulate an external source of fluid, such as supply from microvasculature that is not modeled explicitly. The fluid supply term, $\hat{\varphi}^w$, appears in the mass balance relation for the mixture,

$$\operatorname{div}\left(\mathbf{v}^s + \mathbf{w}\right) = \hat{\varphi}^w \,.$$

$\hat{\varphi}^w$ has units of reciprocal time [$\mathbf{t}^{-1}$]; it represents the rate at which the volume fraction of fluid changes with time.

4.7.3.1 Starling Equation

The material type for Starling's equation for fluid supply is *"Starling"*. The following material parameters need to be defined:

<kp>	hydraulic filtration coefficient, k_p	[**L**^{2}/**F**·**t**]
<pv>	fluid pressure in external source, p_v	[**P**]

The fluid supply is given by Starling's equation,

$$\hat{\varphi}^w = k_p \left(p_v - p \right) ,$$

where p is the fluid pressure in the biphasic material.

Example:

This example defines a fluid supply material of the Starling type.

```
<solvent_supply type="Starling">
  <kp>0.001</kp>
  <pv>0.1</pv>
</solvent_supply>
```

4.8 Biphasic-Solute Materials

Biphasic-solute materials may be used to model the transport of a solvent and a solute in a neutral porous solid matrix, under isothermal conditions. Each of these mixture constituents is assumed to be intrinsically incompressible. This means that their true densities are invariant in space and time; this assumption further implies that a biphasic-solute mixture will undergo zero volume change when subjected to a hydrostatic fluid pressure. Yet the mixture is compressible because the pores of the solid matrix may gain or lose fluid under general loading conditions. Therefore, the constitutive relation of the solid matrix should be chosen from the list of compressible materials provided in Section 4.1.3. The volume fraction of the solute is assumed to be negligible relative to the volume fractions of the solid or solvent. This means that the mixture will not change in volume as the solute concentration changes. As the solute transports through the mixture, it may experience frictional interactions with the solvent and the solid. This friction may act as a hindrance to the solute transport, or may help convect the solute through the mixture. The distinction between frictional exchanges with the solvent and solid is embodied in the specification of two diffusivities for the solute: The free diffusivity, which represents diffusivity in the absence of a solid matrix (frictional exchange only with the solvent) and the mixture diffusivity, which represents the combined frictional interactions with the solvent and solid matrix. The user is referred to the *FEBio Theory Manual* for a more detailed description of the biphasic-solute theory.

Due to steric volume exclusion and short-range electrostatic interactions, the solute may not have access to all of the pores of the solid matrix. In other words, only a fraction κ of the pores is able to accommodate a solute of a particular size ($0 < \kappa \leqslant 1$). Furthermore, the activity γ of the solute (the extent by which the solute concentration influences its chemical potential) may be similarly altered by the surrounding porous solid matrix. Therefore, the combined effects of volume exclusion and attenuation of activity may be represented by the effective solubility $\tilde{\kappa} = \kappa/\gamma$, such that the chemical potential μ of the solute is given by

$$\mu = \mu_0(\theta) + \frac{R\theta}{M} \ln \frac{c}{\tilde{\kappa}} . \tag{4.8.1}$$

In this expression, μ_0 is the solute chemical potential at some reference temperature θ; c is the solute concentration on a solution-volume basis (number of moles of solute per volume of interstitial fluid in the mixture); M is the solute molecular weight (an invariant quantity); and R is the universal gas constant. In a biphasic-solute material, a constitutive relation is needed for $\tilde{\kappa}$; in general, $\tilde{\kappa}$ may be a function of the solid matrix strain and the solute concentration. In FEBio, the dependence of the effective solubility on the solid matrix strain is currently constrained to a dependence on $J = \det \mathbf{F}$.

In a biphasic-solute material, the interstitial fluid pressure p is influenced by both mechanical and chemical environments. In other words, this pressure includes both mechanical and osmotic contributions, the latter arising from the presence of the solute. The solvent mechano-chemical potential $\tilde{\mu}^w$ is given by

$$\tilde{\mu}^w = \mu_0^w(\theta) + \frac{1}{\rho_T^w}(p - R\theta\Phi c) , \tag{4.8.2}$$

where μ_0^w is the solvent chemical potential at some reference temperature θ; ρ_T^w is the true density of the solvent (an invariant property for an intrinsically incompressible fluid); and Φ is the osmotic coefficient which represents the extent by which the solute concentration influences the solvent chemical potential. In a biphasic-solute material, a constitutive relation is needed for Φ; in general, Φ may be a function of the solid matrix strain and the solute concentration. In FEBio, the depen-

dence of the osmotic coefficient on the solid matrix strain is currently constrained to a dependence on $J = \det \mathbf{F}$.

The solute mechano-chemical potential is nearly equal to its chemical potential because the solute volume fraction is assumed to be negligible. In general, momentum and energy balances evaluated across a boundary surface in a biphasic-solute mixture require that the mechano-chemical potentials of solvent and solute be continuous across that surface. These continuity requirements are enforced automatically in FEBio by defining the effective fluid pressure $\tilde{p}$ and solute concentration $\tilde{c}$ as

$$\begin{aligned} \tilde{p} &= p - R\theta\Phi c \\ \tilde{c} &= \frac{c}{\tilde{\kappa}} \end{aligned} \quad . \tag{4.8.3}$$

Therefore, nodal variables in FEBio consist of the solid matrix displacement $\mathbf{u}$, the effective fluid pressure $\tilde{p}$, and the effective solute concentration $\tilde{c}$. Essential boundary conditions must be imposed on these variables, and not on the actual pressure p or concentration c. (In a biphasic material however, since $c = 0$, the effective and actual fluid pressures are the same, $p = \tilde{p}$.)

The mixture stress in a biphasic-solute material is given by $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}^e$, where $\boldsymbol{\sigma}^e$ is the stress arising from the solid matrix strain. The mixture traction on a surface with unit outward normal $\mathbf{n}$ is $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$. This traction is continuous across the boundary surface. Therefore, the corresponding natural boundary condition for a biphasic-solute mixture is $\mathbf{t} = \mathbf{0}$. (In other words, if no boundary condition is imposed on the solid matrix displacement or mixture traction, the natural boundary condition is in effect.)

The natural boundary conditions for the solvent and solute are similarly $\mathbf{w} \cdot \mathbf{n} = 0$ and $\mathbf{j} \cdot \mathbf{n} = 0$, where $\mathbf{w}$ is the volumetric flux of solvent relative to the solid and $\mathbf{j}$ is the molar flux of solute relative to the solid. In general, $\mathbf{w}$ and $\mathbf{j}$ are given by

$$\begin{aligned} \mathbf{w} &= -\tilde{\mathbf{k}} \cdot \left(\nabla\tilde{p} + R\theta \frac{\tilde{\kappa}}{d_0} \mathbf{d} \cdot \nabla\tilde{c} \right) \\ \mathbf{j} &= \tilde{\kappa}\mathbf{d} \cdot \left(-\varphi^w \nabla\tilde{c} + \frac{\tilde{c}}{d_0} \mathbf{w} \right) \end{aligned} \quad , \tag{4.8.4}$$

where

$$\tilde{\mathbf{k}} = \left[\mathbf{k}^{-1} + \frac{R\theta}{\varphi^w} \frac{\tilde{\kappa} c}{d_0} \left(\mathbf{I} - \frac{\mathbf{d}}{d_0} \right) \right]^{-1} \tag{4.8.5}$$

is the effective hydraulic permeability of the interstitial fluid solution (solvent and solute) through the porous solid matrix; $\mathbf{k}$ is the hydraulic permeability of the solvent through the porous solid matrix; $\mathbf{d}$ is the solute diffusivity through the mixture (frictional interactions with solvent and solid); and d_0 is the solute free diffusivity (frictional interactions with solvent only). $\varphi^w \approx 1 - \varphi^s$ is the solid matrix porosity in the current configuration. The above expressions for the solvent and solute flux do not account for external body forces.

The governing equations for a biphasic-solute material are the momentum balance for the mixture, Eq.(4.7.3), the mass balance for the mixture, which reduces to Eq.(4.7.4) under the assumption of dilute solutions, and the mass balance for the solute,

$$\frac{\partial \left(\varphi^w c \right)}{\partial t} + \operatorname{div} \left(\mathbf{j} + \varphi^w c \mathbf{v}^s \right) = 0 \, . \tag{4.8.6}$$

4.8.1 Guidelines for Biphasic-Solute Analyses

4.8.1.1 Prescribed Boundary Conditions

In most analyses, it may be assumed that the ambient fluid pressure in the external environment is zero, thus $p_* = 0$, where the subscripted asterisk is used to denote environmental conditions. The ambient solute concentration may be represented by c_*. It follows that the effective fluid pressure in the external environment is $\tilde{p}_* = -R\theta\Phi_* c_*$ and the effective concentration is $\tilde{c}_* = c_*/\tilde{\kappa}_*$. Therefore, in biphasic-solute analyses, whenever the external environment contains a solute at a concentration of c_*, the user must remember to prescribe non-zero boundary conditions for the effective solute concentration *and* the effective fluid pressure.

Letting $p_* = 0$ also implies that prescribed mixture normal tractions (Section 3.12.2.3) represent only the traction above ambient conditions. Note that users are not obligated to assume that $p_* = 0$. However, if a non-zero value is assumed for the ambient pressure, then users must remember to incorporate this non-zero value whenever prescribing mixture normal tractions.

4.8.1.2 Prescribed Initial Conditions

When a biphasic-solute material is initially exposed to a given external environment with effective pressure $\tilde{p}_*$ and effective concentration $\tilde{c}_*$, the initial conditions inside the material should be set to $\tilde{p} = \tilde{p}_*$ and $\tilde{c} = \tilde{c}_*$ in order to produce the correct initial state. The values of $\tilde{p}_*$ and $\tilde{c}_*$ should be evaluated as described in Section 7.6.2.

4.8.2 General Specification of Biphasic-Solute Materials

The material type for a biphasic-solute material is *"biphasic-solute"*. Constitutive relations must be provided for the solid matrix, the hydraulic permeability $\mathbf{k}$, the solute diffusivities $\mathbf{d}$ and d_0, the effective solubility $\tilde{\kappa}$ and the osmotic coefficient Φ. Therefore, the following parameters must be defined:

<solid>	specification of the solid matrix
<phi0>	solid volume fraction φ_r^s in the reference configuration
<permeability>	specification of the hydraulic permeability $\mathbf{k}$
<osmotic_coefficient>	specification of the osmotic coefficient $\Phi \quad \mathbf{d}d_0$
<solute>	specification of the solute properties

The <solid> tag encloses a description of the solid matrix constitutive relation and associated material properties, as may be selected from the list provided in Section 4.1.3. The solid volume fraction in the reference configuration, <phi0>, must be greater than 0 (no solid) and less than 1 (only solid). The volume fraction of fluid (also known as the porosity) in the reference configuration is given by $1 - \varphi_0$. The <permeability> tag encloses a description of the permeability constitutive relation and associated material properties, as may be selected from the list presented in Section 4.7.2.

The <solute> tag provides a description of the solute in the biphasic-solute mixture. This tag includes the required *sol* attribute, which should reference a solute *id* from the <Solutes> description in the <Globals> section (Section 3.4.2). The following parameters must be defined in this description:

<diffusivity>	specification of the solute diffusivities $\mathbf{d}$ and d_0
<solubility>	specification of the solute effective solubility $\tilde{\kappa}$

The <diffusivity> and <solubility> tags enclose descriptions of materials that may be selected from the lists presented in Sections 4.8.3 and 4.8.4, respectively. Each solute tag must include a "sol" attribute.

Example:

```
<material id="1" name="Biological tissue" type="biphasic-solute">
  <solid name="Elasticity" type="neo-Hookean">
    <E>1.0</E>
    <v>0.3</v>
  </solid>
  <phi0>0.2</phi0>
  <permeability name="Permeability" type="perm-const-iso">
    ... (description of permeability material)
  </permeability>
  <osmotic_coefficient name="Osmotic" type="osm-coef-const">
    ... (description of osmotic coefficient material)
  </osmotic_coefficient>
  <solute sol="1">
    <diffusivity name="Diffusivity" type="diff-const-iso">
      ... (description of diffusivity material)
```

```
      </diffusivity>
      <solubility name="Solubility" type="solub-const">
        ... (description of solubility material)
      </solubility>
    </solute>
  </material>
```

When a biphasic-solute material is employed in an analysis, it is also necessary to specify the values of the universal gas constant R [**F**·**L**/**n**·**T**] and absolute temperature θ [**T**] under <Constants> in the <Globals> section, using a self-consistent set of units. A solute must also be defined in the <Solutes> section, whose id should be associated with the "sol" attribute in the solute material description.

Example:

```
<Globals>
  <Constants>
    <R>8.314</R>
    <T>298</T>
  </Constants>
  <Solutes>
    <solute id="1" name="neutral">
      <charge_number>0</charge_number>
    </solute>
  </Solutes>
</Globals>
```

It is also possible to create models with biphasic-solute materials that use different solutes in different regions. In that case, introduce additional solute entries in the <Solutes> section and refer to those solute ids in the biphasic-solute material descriptions.

4.8.3 Diffusivity Materials

Diffusivity materials provide a constitutive relation for the solute diffusivity in a biphasic-solute material. In general, the diffusivity tensor $\mathbf{d}$ may be a function of strain and solute concentration.

4.8.3.1 Constant Isotropic Diffusivity

The material type for constant isotropic diffusivity materials is "*diff-const-iso"*. The following material parameters must be defined:

<free_diff>	free diffusivity d_0 of solute (diffusivity in solution)	[**L**^{2}/**t**]
<diff>	constant isotropic diffusivity d of solute in biphasic-solute mixture	[**L**^{2}/**t**]

When the permeability is isotropic,

$$\mathbf{d} = d\mathbf{I}$$

For this material model, d is constant. This assumption is only true when strains are small. Note that the user must specify $d \leqslant d_0$, since a solute cannot diffuse through the biphasic-solute mixture faster than in free solution.

Example:

```
<diffusivity name="Permeability" type="diff-const-iso">
  <free_diff>1e-9</ free_diff >
  <diff>0.5e-9</diff>
</diffusivity>
```

4.8.3.2 Constant Orthotropic Diffusivity

The material type for constant orthotropic diffusivity materials is "*diff-const-ortho*". The following material parameters must be defined:

<free_diff>	free diffusivity d_0 of solute (diffusivity in solution)	[**L**^{2}/**t**]
<diff>	diffusivities d^a along orthogonal directions $(a = 1, 2, 3)$	[**L**^{2}/**t**]

When the permeability is orhotropic,

$$\mathbf{d} = \sum_{a=1}^{3} d^a \mathbf{V}_a \otimes \mathbf{V}_a$$

where $\mathbf{V}_a$ are orthonormal vectors normal to the planes of symmetry (defined as described in Section 4.1.1). For this material model, d^a's are constant. Therefore this model should be used only when strains are small. Note that the user must specify $d^a \leqslant d_0$, since a solute cannot diffuse through the biphasic-solute mixture faster than in free solution.

Example:

```
<diffusivity name="Permeability" type="diff-const-ortho">
  <free_diff>0.005</ free_diff >
  <diff>0.002,0.001,0.003</diff>
</diffusivity>
```

4.8.3.3 Referentially Isotropic Diffusivity

The material type for a strain-dependent diffusivity tensor which is isotropic in the reference configuration is *"diff-ref-iso"*. The following material parameters need to be defined:

<free_diff>	free diffusivity d_0	[**L**^{2}/**t**]
<diff0>	diffusivity d_{0r}	[**L**^{2}/**t**]
<diff1>	diffusivity d_{1r}	[**L**^{2}/**t**]
<diff2>	diffusivity d_{2r}	[**L**^{2}/**t**]
<M>	exponential strain-dependence coefficient M ($M \geqslant 0$)	[ ]
<alpha>	power-law exponent α ($\alpha \geqslant 0$)	[ ]

This material uses a strain-dependent diffusivity tensor that accommodates strain-induced anisotropy:

$$\mathbf{d} = \left(d_{0r}\mathbf{I} + \frac{d_{1r}}{J^2}\mathbf{b} + \frac{d_{2r}}{J^4}\mathbf{b}^2 \right) \left(\frac{J - \varphi_r^s}{1 - \varphi_r^s} \right) e^{M\left(J^2-1\right)/2},$$

where $J$is the jacobian of the deformation, i.e. $J = \det \mathbf{F}$ where $\mathbf{F}$ is the deformation gradient, and $\mathbf{b} = \mathbf{F} \cdot \mathbf{F}^T$ is the left Cauchy-Green tensor. Note that the diffusivity in the reference state ($\mathbf{F} = \mathbf{I}$) is isotropic and given by $\mathbf{d} = (d_{0r} + d_{1r} + d_{2r})\,\mathbf{I}$.

Example:

```
<diffusivity name="Diffusivity" type="diff-ref-iso">
  <phi0>0.2</phi0>
  <free_diff>0.005</free_diff>
  <diff0>0.001</diff0>
  <diff1>0.005</diff1>
  <diff2>0.002</diff2>
  <M>1.5</M>
  <alpha>2</alpha>
</diffusivity>
```

4.8.3.4 Referentially Orthotropic Diffusivity

The material type for a strain-dependent diffusivity which is orthotropic in the reference configuration is *"diff-ref-ortho"*. The following material parameters need to be defined:

<free_diff>	free diffusivity d_0	[**L**^{2}/**t**]
<diff0>	isotropic diffusivity d_{0r}	[**L**^{2}/**t**]
<diff1>	diffusivities d^a_{1r} along orthogonal directions ($a = 1, 2, 3$)	[**L**^{2}/**t**]
<diff2>	diffusivities d^a_{2r} along orthogonal directions ($a = 1, 2, 3$)	[**L**^{2}/**t**]
<M0>	isotropic exponential strain-dependence coefficient M_0 ($M_0 \geqslant 0$)	[ ]
<M>	orthotropic exponential strain-dependence coefficient M_a ($a = 1, 2, 3$, $M_a \geqslant 0$)	[ ]
<alpha0>	isotropic power-law exponent α_0 ($\alpha_0 \geqslant 0$)	[ ]
<alpha>	power-law exponent α_a ($a = 1, 2, 3$, $\alpha_a \geqslant 0$)	[ ]

This material uses a strain-dependent diffusivity tensor that accommodates strain-induced anisotropy:

$$\mathbf{d} = d_0\mathbf{I} + \sum_{a=1}^{3} d_1^a \mathbf{m}_a + d_2^a \left(\mathbf{m}_a \cdot \mathbf{b} + \mathbf{b} \cdot \mathbf{m}_a\right),$$

where,

$$d_0 = d_{0r}\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_0} e^{M_0\left(J^2-1\right)/2}$$
$$d_1^a = \frac{d_{1r}^a}{J^2}\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_a} e^{M_a\left(J^2-1\right)/2}, \quad a = 1, 2, 3$$
$$d_2^a = \frac{d_{2r}^a}{2J^4}\left(\frac{J-\varphi_r^s}{1-\varphi_r^s}\right)^{\alpha_a} e^{M_a\left(J^2-1\right)/2}$$

J is the Jacobian of the deformation, i.e. $J = \det \mathbf{F}$ where $\mathbf{F}$ is the deformation gradient. $\mathbf{m}_a$ are second order tensors representing the spatial structural tensors describing the orthogonal planes of symmetry, given by

$$\mathbf{m}_a = \mathbf{F} \cdot (\mathbf{V}_a \otimes \mathbf{V}_a) \cdot \mathbf{F}^T, \quad a = 1 - 3,$$

where $\mathbf{V}_a$ are orthonormal vectors normal to the planes of symmetry (defined as described in Section 4.1.1). Note that the diffusivity in the reference state ($\mathbf{F} = \mathbf{I}$) is given by $\mathbf{d} = d_{0r}\mathbf{I} + \sum_{a=1}^{3} \left(d_{1r}^a + d_{2r}^a\right) \mathbf{V}_a \otimes \mathbf{V}_a$.

Example:

```
<diffusivity name="Diffusivity" type="diff-ref-ortho">
  <phi0>0.2</phi0>
  <free_diff>0.005</free_diff>
  <diff00>0.001</diff00>
  <diff1>0.01, 0.02, 0.03</diff1>
  <diff2>0.001, 0.002, 0.003</diff2>
  <M0>0.5</M0>
```

```
    <M>1.5, 2.0, 2.5</M>
    <alpha0>1.5</alpha0>
    <alpha>2, 2.5, 3</alpha>
  </diffusivity>
```

4.8.3.5 Albro Isotropic Diffusivity

The material type for a porosity and concentration-dependent diffusivity which is isotropic is *"diff-Albro-iso"*. The following material parameters need to be defined:

<free_diff>	free diffusivity d_0	[**L**^{2}/**t**]
<cdinv>	inverse of characteristic concentration for concentration-dependence c_D^{-1}	[**L**^{3}/**n**]
<alphad>	coefficient of porosity-dependence α_D	[ ]

This material uses a porosity and concentration-dependent diffusivity tensor that remains isotropic with deformation:

$$\mathbf{d} = d_0 \exp\left(-\alpha_D \frac{1-\varphi^w}{\varphi^w} - \frac{c}{c_D}\right)\mathbf{I},$$

where $c_D^{-1} = 1/c_D$ and the porosity φ^w varies with deformation according to the kinematic constraint

$$\varphi^w = 1 - \frac{\varphi_r^s}{J}\,.$$

J is the Jacobian of the deformation, i.e. $J = \det \mathbf{F}$ where $\mathbf{F}$ is the deformation gradient and φ_r^s is the referential solid volume fraction. Here, c represents the actual concentration of the solute whose diffusivity is given by $\mathbf{d}$. This constitutive relation is based on the experimental findings reported by Albro et al. [1].

Example:

```
<solute sol="1">
  <diffusivity type="diff-Albro-iso">
    <free_diff>123e-6</free_diff>
    <alphad>18</alphad>
    <cdinv>0.0625</cdinv>
  </diffusivity>
  <solubility type="solub-const">
    <solub>1</solub>
  </solubility>
</solute>
```

4.8.4 Solubility Materials

4.8.4.1 Constant Solubility

The material type for constant solubility materials is "*solub-const*". The following material parameters must be defined:

<solub>	solubility $\tilde{\kappa}$	[ ]

For this material model, $\tilde{\kappa}$ is constant.
Example:

```
<solubility name="Solubility" type="solub-const">
  <solub>1</solub>
</solubility>
```

4.8.5 Osmotic Coefficient Materials

4.8.5.1 Constant Osmotic Coefficient

The material type for constant osmotic coefficient materials is "*osm-coef-const*". The following material parameters must be defined:

<osmcoef>	Osmotic coefficient Φ	[ ]

For this material model, Φ is constant.
Example:

```
<osmotic_coefficient name="Osmotic coefficient" type="osm-coef-const">
  <osmcoef>1</osmcoef>
</osmotic_coefficient>
```

4.9 Triphasic and Multiphasic Materials

Triphasic materials may be used to model the transport of a solvent and a pair of monovalent salt counter-ions (two solutes with charge numbers $+1$ and -1) in a charged porous solid matrix, under isothermal conditions. Multiphasic materials may be used to model the transport of a solvent and any number of neutral or charged solutes; a triphasic mixture is a special case of a multiphasic mixture. Each of the mixture constituents is assumed to be intrinsically incompressible. This means that their true densities are invariant in space and time; this assumption further implies that a multiphasic mixture will undergo zero volume change when subjected to a hydrostatic fluid pressure. Yet the mixture is compressible because the pores of the solid matrix may gain or lose fluid under general loading conditions. Therefore, the constitutive relation of the solid matrix should be chosen from the list of compressible materials provided in Section 4.1.3. The volume fraction of the solutes is assumed to be negligible relative to the volume fractions of the solid or solvent. This means that the mixture will not change in volume as the solute concentrations change. As the solutes transport through the mixture, they may experience frictional interactions with the solvent and the solid. This friction may act as a hindrance to the solute transport, or may help convect the solutes through the mixture. The distinction between frictional exchanges with the solvent and solid is embodied in the specification of two diffusivities for each solute: The free diffusivity, which represents diffusivity in the absence of a solid matrix (frictional exchange only with the solvent) and the mixture diffusivity, which represents the combined frictional interactions with the solvent and solid matrix. The user is referred to the *FEBio Theory Manual* for a more detailed description of triphasic and multiphasic theory.

Due to steric volume exclusion and short-range electrostatic interactions, a solute α may not have access to all of the pores of the solid matrix. In other words, only a fraction κ^α of the pores is able to accommodate solute α ($0 < \kappa^\alpha \leqslant 1$). Furthermore, the activity γ^α of solute α (the extent by which the solute concentration influences its chemical potential) may be similarly altered by the surrounding porous solid matrix. Therefore, the combined effects of volume exclusion and attenuation of activity may be represented by the effective solubility $\hat{\kappa}^\alpha = \kappa^\alpha/\gamma^\alpha$, such that the chemical potential μ of the solute is given by

$$\mu^\alpha = \mu_0^\alpha(\theta) + \frac{R\theta}{M^\alpha}\ln\frac{c^\alpha}{\hat{\kappa}^\alpha}\,. \tag{4.9.1}$$

In this expression, μ_0^α is the solute chemical potential at some reference temperature θ; c^α is the solute concentration on a solution-volume basis (number of moles of solute per volume of interstitial fluid in the mixture); M^α is the solute molecular weight (an invariant quantity); and R is the universal gas constant. In a triphasic material, a constitutive relation is needed for $\hat{\kappa}^\alpha$; in general, $\hat{\kappa}^\alpha$ may be a function of the solid matrix strain and the solute concentration. In FEBio, the dependence of the effective solubility on the solid matrix strain is currently constrained to a dependence on $J = \det\mathbf{F}$.

The solid matrix of a multiphasic material may be charged and its charge density is given by c^F. This charge density may be either negative or positive. The charge density varies with the deformation, increasing when the pore volume decreases. Based on the balance of mass for the solid,

$$c^F = \frac{1-\varphi_r^s}{J-\varphi_r^s}c_r^F\,, \tag{4.9.2}$$

where φ_r^s is the solid volume fraction and c_r^F is the fixed charge density in the reference configuration.

In the multiphasic theory it is assumed that electroneutrality is satisfied at all times. In other words, the net charge of the mixture is always zero (neutral). This electroneutrality condition is represented by a constraint equation on the ion concentrations,

$$c^F + \sum_\alpha z^\alpha c^\alpha = 0\,, \tag{4.9.3}$$

where z^α is the charge number of solute $\alpha z^- = -1$. Since the concentrations of the cation and anion inside the triphasic material are not the same, an electrical potential difference is produced between the interstitial and external environments. The electric potential in the triphasic mixture is denoted by ψ and its effect combines with the chemical potential of each solute to produce the electrochemical potential $\tilde{\mu}^\alpha$, where

$$\tilde{\mu}^\alpha = \mu_0^\alpha(\theta) + \frac{R\theta}{M^\alpha}\ln\frac{c^\alpha}{\hat{\kappa}^\alpha} + \frac{z^\alpha}{M^\alpha}F_c\psi\,. \tag{4.9.4}$$

In this expression, F_c represents Faraday's constant. It is also possible to rearrange this expression as

$$\tilde{\mu}^\alpha = \mu_0^\alpha(\theta) + \frac{R\theta}{M^\alpha}\ln\left[\exp\left(z^\alpha\frac{F_c\psi}{R\theta}\right)\frac{c^\alpha}{\hat{\kappa}^\alpha}\right]\,. \tag{4.9.5}$$

In a multiphasic material, the interstitial fluid pressure p is influenced by both mechanical and chemical environments. In other words, this pressure includes both mechanical and osmotic contributions, the latter arising from the presence of the solutes. The solvent mechano-chemical potential $\tilde{\mu}^w$ is given by

$$\tilde{\mu}^w = \mu_0^w(\theta) + \frac{1}{\rho_T^w}\left(p - R\theta\Phi\sum_\alpha c^\alpha\right)\,, \tag{4.9.6}$$

where μ_0^w is the solvent chemical potential at some reference temperature θ; ρ_T^w is the true density of the solvent (an invariant property for an intrinsically incompressible fluid); and Φ is the osmotic coefficient which represents the extent by which the solute concentrations influence the solvent chemical potential. In a multiphasic material, a constitutive relation is needed for Φ; in general, Φ may be a function of the solid matrix strain and the solute concentrations. In FEBio, the dependence of the osmotic coefficient on the solid matrix strain is currently constrained to a dependence on $J = \det\mathbf{F}$.

The solute mechano-electrochemical potential is nearly equal to its electrochemical potential because the solute volume fraction is assumed to be negligible. The solvent mechano-electrochemical potential is the same as its mechano-chemical potential, since the solvent is neutral in a multiphasic mixture. In general, momentum and energy balances evaluated across a boundary surface in a multiphasic mixture require that the mechano-electrochemical potentials of solvent and solutes be continuous across that surface. These continuity requirements are enforced automatically in FEBio by defining the effective fluid pressure $\tilde{p}$ and solute concentration $\tilde{c}^\alpha$ as

$$\begin{aligned}\tilde{p} &= p - R\theta\Phi\textstyle\sum_\alpha c^\alpha\\ \tilde{c}^\alpha &= c^\alpha/\tilde{\kappa}^\alpha\end{aligned}\,, \tag{4.9.7}$$

where

$$\tilde{\kappa}^\alpha = \hat{\kappa}^\alpha\exp\left(-z^\alpha\frac{F_c\psi}{R\theta}\right) \tag{4.9.8}$$

is the partition coefficient for solute α. The partition coefficient incorporates the combined effects of solubility and long-range electrostatic interactions to determine the ratio of interstitial to external concentration for that solute. Therefore, the effective concentration represents a measure of the *activity* of the solute, as understood in chemistry. The effective fluid pressure represents that part of the pressure which is over and above osmotic effects.

In FEBio, nodal variables consist of the solid matrix displacement $\mathbf{u}$, the effective fluid pressure $\tilde{p}$, and the effective solute concentrations $\tilde{c}^\alpha$. Essential boundary conditions must be imposed on these variables, and not on the actual pressure p or concentrations c^α. (In a biphasic material however, since $c^\alpha = 0$, the effective and actual fluid pressures are the same, $p = \tilde{p}$.)

The mixture stress in a triphasic material is given by $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}^e$, where $\boldsymbol{\sigma}^e$ is the stress arising from the solid matrix strain. The mixture traction on a surface with unit outward normal $\mathbf{n}$ is $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$. This traction is continuous across the boundary surface. Therefore, the corresponding natural boundary condition for a multiphasic mixture is $\mathbf{t} = \mathbf{0}$. (In other words, if no boundary condition is imposed on the solid matrix displacement or mixture traction, the natural boundary condition is in effect.)

The natural boundary conditions for the solvent and solutes are similarly $\mathbf{w}\cdot\mathbf{n} = 0$ and $\mathbf{j}^\alpha\cdot\mathbf{n} = 0$, where $\mathbf{w}$ is the volumetric flux of solvent relative to the solid and $\mathbf{j}^\alpha$ is the molar flux of solute α relative to the solid. In general, $\mathbf{w}$ and $\mathbf{j}^\alpha$ are given by

$$\begin{aligned} \mathbf{w} &= -\tilde{\mathbf{k}} \cdot \left(\nabla\tilde{p} + R\theta \sum_\alpha \frac{\tilde{\kappa}^\alpha}{d_0^\alpha} \mathbf{d}^\alpha \cdot \nabla\tilde{c}^\alpha \right), \\ \mathbf{j}^\alpha &= \tilde{\kappa}^\alpha\, \mathbf{d}^\alpha \cdot \left(-\varphi^w \nabla\tilde{c}^\alpha + \frac{\tilde{c}^\alpha}{d_0^\alpha}\mathbf{w} \right), \end{aligned} \tag{4.9.9}$$

where

$$\tilde{\mathbf{k}} = \left[\mathbf{k}^{-1} + \frac{R\theta}{\varphi^w} \sum_\alpha \frac{\tilde{\kappa}^\alpha c^\alpha}{d_0^\alpha} \left(\mathbf{I} - \frac{\mathbf{d}^\alpha}{d_0^\alpha} \right) \right]^{-1} \tag{4.9.10}$$

is the effective hydraulic permeability of the interstitial fluid solution (solvent and solutes) through the porous solid matrix; $\mathbf{k}$ is the hydraulic permeability of the solvent through the porous solid matrix; $\mathbf{d}^\alpha$ is the diffusivity of solute α through the mixture (frictional interactions with solvent and solid); and d_0^α is its free diffusivity (frictional interactions with solvent only). $\varphi^w \approx 1 - \varphi^s$ is the solid matrix porosity in the current configuration. The above expressions for the solvent and solute flux do not account for external body forces.

Also see Section 7.6 for additional guidelines for running multiphasic materials.

4.9.1 Guidelines for Multiphasic Analyses

4.9.1.1 Initial State of Swelling

Under traction-free conditions, a multiphasic material is usually in a state of swelling due to the osmotic pressure difference between the interstitial fluid and the external environment. This osmotic pressure arises from the difference in interstitial versus external concentrations of cations and anions, caused by the charged solid matrix and the requirement to satisfy electroneutrality. An osmotic pressure difference arising from such electrostatic interactions is known as the *Donnan osmotic pressure*. When the Donnan pressure is non-zero, traction-free conditions do not produce stress-free conditions for the solid matrix, since the matrix must expand until its stressed state resists the swelling pressure.

The Donnan pressure reduces to zero when the fixed charged density is zero, or when the external environment is infinitely hypertonic (having ion concentrations infinitely greater than the interstitial fixed charge density). Since these two conditions represent special cases, it is generally necessary to devise methods for achieving the desired initial state of swelling, in an analysis where loads or displacements need to be prescribed over and above this swollen state. Swelling occurs as a result of the influx of solvent into the porous solid matrix. This influx is a time-dependent process that could require extensive analysis time. Therefore, it is computationally efficacious to achieve the initial state of swelling by using a multi-step analysis (Chapter 5.6.2) where the first step is a steady-state analysis (Section 3.3.1). In this steady-state step, the fixed charge density may be ramped up from zero to the desired value using a load curve for that property or, alternatively, the external environmental conditions may be reduced from a very high hypertonic state down to the desired level. In the second step, prescribed displacement boundary conditions (when needed) may be specified to be of type *relative* (Section 3.10.1), so that they become superposed over and above the initial swelling state.

Example:

```
<Step>
  <Module type="multiphasic"/>
  <Control>
    <analysis type="steady-state"/>
    ...
  </Control>
</Step>
<Step>
  <Module type="multiphasic"/>
  <Control>
    ...
  </Control>
  <Boundary>
    <prescribe type="relative">
      <node id="22" bc="z" lc="4">1</node>
      ...
    </prescribe>
  </Boundary>
</Step>
```

4.9.1.2 Prescribed Boundary Conditions

In most analyses, it may be assumed that the ambient fluid pressure and electric potential in the external environment are zero, thus $p_* = 0$ and $\psi_* = 0$, where the subscripted asterisk is used to denote environmental conditions. Since the external environment does not include a solid matrix, the fixed charge density there is zero. For example, in a triphasic analysis, $c_*^+ = c_*^- \equiv c_*$. It follows that the effective fluid pressure in the external environment is $\tilde{p}_* = -R\theta\Phi_* \sum_\alpha c_*^\alpha$ and the effective concentrations are $\tilde{c}_*^\alpha = c_*^\alpha/\hat{\kappa}_*^\alpha \tilde{c}_*^\alpha$. Therefore, in multiphasic analyses, whenever the external environment contains solutes with non-zero concentrations c_*^α, the user must remember to prescribe non-zero boundary conditions for the effective solute concentrations *and* the effective fluid pressure.

Letting $p_* = 0$ also implies that prescribed mixture normal tractions (Section 3.12.2.3) represent only the traction above ambient conditions. Note that users are not obligated to assume that $p_* = 0$. However, if a non-zero value is assumed for the ambient pressure, then users must remember to incorporate this non-zero value whenever prescribing mixture normal tractions. Similarly, users are not required to assume that $\psi_* = 0$; when a non-zero value is assumed for the electric potential of the external environment, the prescribed boundary conditions for the effective concentrations should be evaluated using the corresponding partition coefficient, $\tilde{c}_*^\alpha = c_*^\alpha/\tilde{\kappa}_*^\alpha \tilde{c}_*^\alpha$.

4.9.1.3 Prescribed Initial Conditions

When a multiphasic material is initially exposed to a given external environment with effective pressure $\tilde{p}_*$ and effective concentrations $\tilde{c}_*^\alpha$, the initial conditions inside the material should be set to $\tilde{p} = \tilde{p}_*$ and $\tilde{c}^\alpha = \tilde{c}_*^\alpha$ in order to expedite the evaluation of the initial state of swelling. The values of $\tilde{p}_*$ and $\tilde{c}_*^\alpha$ should be evaluated as described in Section 7.6.2.

4.9.1.4 Prescribed Effective Solute Flux

The finite element formulation for multiphasic materials in FEBio requires that the natural boundary condition for solute α be prescribed as $\tilde{j}_n^\alpha \equiv j_n^\alpha + \sum_\beta z^\beta j_n^\beta$, where $\tilde{j}_n^\alpha$ is the effective solute flux. For a mixture containing only neutral solutes ($z^\beta = 0, \forall\beta$), it follows that $\tilde{j}_n^\alpha = j_n^\alpha$.

4.9.1.5 Prescribed Electric Current Density

The electric current density in a mixture is a linear superposition of the ion fluxes,

$$\mathbf{I}_e = F_c \sum_\alpha z^\alpha \mathbf{j}^\alpha \,. \tag{4.9.11}$$

Since only the normal component $j_n^\alpha = \mathbf{j}^\alpha \cdot \mathbf{n}$ of ion fluxes may be prescribed at a boundary, it follows that only the normal component $I_n = \mathbf{I}_e \cdot \mathbf{n}$ of the current density may be prescribed. To prescribe I_n, it is necessary to know the nature of the ion species in the mixture, and how the current is being applied. For example, if the ions in the triphasic mixture consist of Na^+ and Cl^-, and if the current is being applied using silver/silver chloride (Ag/AgCl) electrodes, a chemical reaction occurs at the anode where Ag combines with Cl^- to produce AgCl, donating an electron to the electrode to transport the current. At the cathode, the reverse process takes place. Therefore, in this system, there is only flux of Cl^- and no flux of Na^+ ($j_n^+ = 0$) at the electrode-mixture interface, so that the prescribed boundary condition should be $j_n^- = -I_n/F_c$.

Since $z^+ = +1$ and $z^- = -1$ in a triphasic mixture, the corresponding effective fluxes are given by $\tilde{j}_n^+ = 2j_n^+ - j_n^- = I_n/F_c$ and $\tilde{j}_n^- = j_n^+ = 0$.

4.9.1.6 Electrical Grounding

If a multiphasic mixture containing ions is completely surrounded by ion-impermeant boundaries it is necessary to ground the mixture to prevent unconstrained fluctuations of the electric potential. Grounding is performed by prescribing the effective concentration of one or more ions, at a location inside the mixture or on one of its boundaries corresponding to the location of the grounding electrode. The choice of ion(s) to constrain may be guided by the type of grounding electrode and the reference electrolyte bath in which it is inserted.

4.9.2 General Specification of Multiphasic Materials

The material type for a multiphasic material is "*multiphasic*". Constitutive relations must be provided for the solid matrix, the mixture fixed charge density, the hydraulic permeability $\mathbf{k}$, the osmotic coefficient Φ, and the properties of each solute: the solute diffusivity in the mixture $\mathbf{d}^\alpha$, the solute free diffusivity d_0^α, and the solute effective solubility $\hat{\kappa}^\alpha$. Therefore, the following parameters must be defined:

<solid>	specification of the solid matrix	
<phi0>	solid volume fraction φ_r^s in the reference configuration	[ ]
<fixed_charge_density>	fixed charge density c_r^F in the reference configuration	[**n**/**L**^{3}]
<permeability>	specification of the hydraulic permeability $\mathbf{k}$	
<solvent_supply>	specification of the solvent supply $\hat{\varphi}^w$	
<osmotic_coefficient>	specification of the osmotic coefficient Φ	
<solute>	specification of the solute properties	
<solid_bound>	specification of solid-bound molecule	

The <solid> tag encloses a description of the solid matrix constitutive relation and associated material properties, as may be selected from the list provided in Section 4.1.3. The solid volume fraction in the reference configuration, <phi0>, must be greater than 0 (no solid) and less than 1 (only solid). The volume fraction of fluid (also known as the porosity) in the reference configuration is given by $1 - \varphi_0$. The <fixed_charge_density> may be negative, positive, or zero. The <permeability> and <osmotic_coefficient> tags enclose descriptions of the permeability and osmotic coefficient constitutive relations and their associated material properties, as may be selected from the list presented in Sections 4.7.2 and 4.8.5.

The optional <solute> tag provides a description of each solute in the multiphasic mixture. Multiple solutes may be defined. Each tag includes the required *sol* attribute, which should reference a solute *id* from the <Solutes> description in the <Globals> section (Section 3.4.2). The following parameters must be defined in this description:

<diffusivity>	specification of the solute diffusivities $\mathbf{d}^\alpha$ and d_0^α
<solubility>	specification of the solute effective solubility $\hat{\kappa}^\alpha$

The <diffusivity> and <solubility> tags enclose descriptions of materials that may be selected from the lists presented in Sections 4.8.3 and 4.8.4, respectively. Each solute tag must include a "sol" attribute

The optional <solid_bound> tag specifies which solid-bound molecule should be included in the multiphasic mixture. Multiple solid-bound molecules may be specified. Each tag should include the required *sbm* attribute, which references an *id* from the <SolidBoundMolecules> description in the <Globals> section (Section 3.4.3). The following parameter must be defined in this description:

<rho0>	initial value of the referential apparent density of the solid-bound molecule ρ_r^σ	[**M**/**L**^{3}]
<rhomin>	optional minimum allowable value of ρ_r^σ (zero by default)	[**M**/**L**^{3}]
<rhomax>	optional maximum allowable value of ρ_r^σ (none by default)	[**M**/**L**^{3}]

If a chemical reaction involves this solid-bound molecule its referential apparent density may evolve over time. The user may place lower and upper bounds on the allowable range of an evolving ρ_r^σ.

Example:

```
<material id="2" name="Media" type="multiphasic">
  <phi0>0.2</phi0>
  <fixed_charge_density>-40</fixed_charge_density>
  <solid name="Solid Matrix" type="Holmes-Mow">
    <density>1</density>
    <E>0.28</E>
    <v>0</v>
    <beta>0</beta>
  </solid>
  <permeability name="Permeability" type="perm-Holmes-Mow">
    <perm>1e-3</perm>
    <M>0</M>
    <alpha>0</alpha>
  </permeability>
  <osmotic_coefficient name="Ideal" type="osm-coef-const">
    <osmcoef>1.0</osmcoef>
  </osmotic_coefficient>
  <solute sol="1">
    <diffusivity name="Diffusivity" type="diff-const-iso">
      <free_diff>1e-3</free_diff>
      <diff>1e-3</diff>
    </diffusivity>
    <solubility name="Solubility" type="solub-const">
      <solub>1.0</solub>
    </solubility>
  </solute>
  <solute sol="2">
    <diffusivity name="Diffusivity" type="diff-const-iso">
      <free_diff>1e-3</free_diff>
      <diff>1e-3</diff>
    </diffusivity>
    <solubility name="Solubility" type="solub-const">
      <solub>1.0</solub>
    </solubility>
  </solute>
</material>
```

When a multiphasic material is employed in an analysis, it is also necessary to specify the values of the universal gas constant R [**F**·**L**/**n**·**T**], absolute temperature θ [**T**], and Faraday's constant F_c [**Q**/**n**] in the <Globals> section, using a self-consistent set of units.

Example:

```
<Globals>
```

```
  <Constants>
    <R>8.314e-6</R>
    <T>298</T>
    <Fc>96500e-9</Fc>
  </Constants>
  <Solutes>
    <solute id="1" name="Na">
      <charge_number>1</charge_number>
    </solute>
    <solute id="2" name="Cl">
      <charge_number>-1</charge_number>
    </solute>
  </Solutes>
</Globals>
```

Example:

Self-consistent units for a triphasic analysis	
Primary Units	
time	s
length	mm
force	N
mole	nmol
charge	C
temperature	K
Derived Units	
stress	N/mm^2, MPa
permeability	mm^4/N·s, mm^2/MPa ·s
diffusivity	mm^2/s
concentration	nmol/mm^3, mM
charge density	nEq/mm^3, mEq/L
voltage	mV
current density	A/mm^2
current	A

It is also possible to create models with multiphasic materials that use different solutes in different regions. In that case, introduce additional solute entries in the <Solutes> section and refer to those solute ids in the multiphasic material descriptions. Generally, two adjoining multiphasic regions may share the same solute (e.g., Na in both regions), in which case that solute may transport freely across the interface separating these regions; or they may share no solute, in which case the interface is impermeable to all solutes.

4.9.3 Solvent Supply Materials

Solvent supply materials may be used to simulate an external source of solvent, such as supply from microvasculature that is not modeled explicitly. The solvent supply term, $\hat{\varphi}^w$, appears in the mass balance relation for the mixture,

$$\operatorname{div}\left(\mathbf{v}^s + \mathbf{w}\right) = \hat{\varphi}^w \,. \tag{4.9.12}$$

$\hat{\varphi}^w$ has units of reciprocal time [$\mathbf{t}^{-1}$]; it represents the rate at which the volume fraction of solvent changes with time.

4.9.3.1 Starling Equation

The material type for Starling's equation for fluid supply is *"Starling"*. The following material parameters need to be defined:

<kp>	hydraulic filtration coefficient, k_p	[**L**^{2}/**F**·**t**]
<pv>	effective fluid pressure in external source, $\tilde{p}_v$	[**P**]
<qc sol="n">	osmotic filtration coefficient, q_c^α	[**L**^{3}/**n**·**t**]
<cv sol="n">	effective solute concentration in external source, $\tilde{c}_v^\alpha$	[**n**/**L**^{3}]

The fluid supply is given by Starling's equation,

$$\hat{\varphi}^w = k_p \left(\tilde{p}_v - \tilde{p}\right) + \sum_\alpha q_c^\alpha \left(\tilde{c}_v^\alpha - \tilde{c}^\alpha\right) ,$$

where $\tilde{p}$ is the effective fluid pressure in the multiphasic material.

Example:

This example defines a solvent supply material of the Starling type for a multiphasic mixture containing one solute.

```
<solvent_supply type="Starling">
  <kp>0.001</kp>
  <pv>0.1</pv>
  <qc sol="1">1e-5</qc>
  <cv sol="1">150</cv>
</solvent_supply>
```

4.10 Chemical Reactions

The following sections describe FEBio's formulation for analyzing mechanochemical events in neutral or charged deformable porous media under finite deformation. The formulation allows full coupling of mechanical and chemical effects, providing a framework where material properties and response functions may depend on solid matrix strain as well as solute concentration.

If you use these capabilities in your published research, we request that you cite the following publication describing its development [8].

4.10.1 Guidelines for Chemical Reaction Analyses

Chemical reactions may be modeled within a multiphasic mixture. The reaction may involve solutes ($\alpha = \iota$) and solid-bound molecules ($\alpha = \sigma$) that move with the solid matrix ($\mathbf{v}^\sigma = \mathbf{v}^s, \forall\sigma$). Consider a general chemical reaction,

$$\sum_\alpha \nu_R^\alpha \mathcal{E}^\alpha \rightarrow \sum_\alpha \nu_P^\alpha \mathcal{E}^\alpha, \tag{4.10.1}$$

where $\mathcal{E}^\alpha$ is the chemical species representing constituent α in the mixture; ν_R^α and ν_P^α represent stoichiometric coefficients of the reactants and products, respectively. To maintain consistency with classical chemical kinetics, the analysis of chemical reactions employs molar concentrations c^α and molar supplies $\hat{c}^\alpha$ on a solution-volume basis for all reactants and products, whether they are solutes or solid-bound molecular species.

Since the molar supply of reactants and products is constrained by stoichiometry, it follows that all molar supplies $\hat{c}^\alpha$ in a specific chemical reaction may be related to a *molar production rate* $\hat{\zeta}$ according to

$$\hat{c}^\alpha = \nu^\alpha \hat{\zeta}\,, \tag{4.10.2}$$

where ν^α represents the net stoichiometric coefficient for $\mathcal{E}^\alpha$,

$$\nu^\alpha = \nu_P^\alpha - \nu_R^\alpha. \tag{4.10.3}$$

Thus, formulating constitutive relations for $\hat{c}^\alpha$ is equivalent to providing a single relation for $\hat{\zeta}\,(\theta, \mathbf{F}, c^\alpha)$. When the chemical reaction is reversible,

$$\sum_\alpha \nu_R^\alpha \mathcal{E}^\alpha \rightleftharpoons \sum_\alpha \nu_P^\alpha \mathcal{E}^\alpha, \tag{4.10.4}$$

the relations of (4.10.2)-(4.10.3) still apply but the constitutive relation for $\hat{\zeta}$ would be different.

Example:

Consider the dissociation of $CaCl_2$ into ions Ca^{2+} and Cl^-,

$$CaCl_2 \rightleftharpoons Ca^{2+} + 2Cl^-.$$

The mixture contains three constituents. The stoichiometric coefficients of the reactants are $\nu_R^{CaCl_2} = 1$, $\nu_R^{Ca^{2+}} = 0$, $\nu_R^{Cl^-} = 0$, and those of the products are $\nu_P^{CaCl_2} = 0$, $\nu_P^{Ca^{2+}} = 1$, $\nu_P^{Cl^-} = 2$.

The reaction production rate $\hat{\zeta}$ enters into the governing equations of multiphasic mixtures via the mass balance relation for each solute,

$$\frac{1}{J}\frac{D^s\left[J\left(1-\varphi^s\right)c^\iota\right]}{Dt} + \operatorname{div}\mathbf{j}^\iota = \left(1-\varphi^s\right)\nu^\iota\hat{\zeta}\,, \tag{4.10.5}$$

the mass balance for the mixture,

$$\operatorname{div}\left(\mathbf{v}^s + \mathbf{w}\right) = \left(1 - \varphi^s\right)\hat{\zeta}\overline{\mathcal{V}}\,, \tag{4.10.6}$$

where $\overline{\mathcal{V}} = \sum_\alpha \nu^\alpha \mathcal{V}^\alpha$ and $\mathcal{V}^\alpha = M^\alpha/\rho_T^\alpha$ is the molar volume of α, and the mass balance for solid-bound constituents,

$$D^s\rho_r^\sigma/Dt = \hat{\rho}_r^\sigma\,, \tag{4.10.7}$$

where ρ_r^σ is the referential apparent mass density (mass of σ per mixture volume in the reference configuration), and $\hat{\rho}_r^\sigma$ is the referential apparent mass supply of solid constituent σ, related to molar concentrations and supplies via

$$c^\sigma = \frac{\rho_r^\sigma}{\left(J - \varphi_r^s\right)M^\sigma}, \quad \hat{c}^\sigma = \frac{\hat{\rho}_r^\sigma}{\left(J - \varphi_r^s\right)M^\sigma}\,. \tag{4.10.8}$$

Internally, the content of solid-bound species is stored in ρ_r^σ and (4.10.8) is used to evaluate c^σ when needed for the calculation of $\hat{\zeta}$. If a solid-bound molecule is involved in a chemical reaction, equation (4.10.7) is integrated to produce an updated value of ρ_r^σ, using $\hat{\rho}_r^\sigma = \left(J - \varphi_r^s\right)M^\sigma\nu^\sigma\hat{\zeta}$ based on (4.10.2) and (4.10.8).

Evolving solid content due to chemical reactions implies that the referential solid volume fraction φ_r^s may not remain constant. This value is updated at every time point using

$$\varphi_r^s = \varphi_0^s + \sum_\sigma \frac{\rho_r^\sigma}{\rho_T^\sigma}\,, \tag{4.10.9}$$

where φ_0^s is the solid volume fraction specified by the multiphasic material parameter *phi0* (Section 4.9.2). Thus, φ_0^s may be used to account for the solid volume fraction not contributed explicitly by solid-bound molecules. Based on kinematics, the solid volume fraction in the current configuration is given by $\varphi^s = \varphi_r^s/J$. Therefore, since $0 \leqslant \varphi^s \leqslant 1$ by definition, it follows that $0 \leqslant \varphi_r^s \leqslant J$, implying that the referential solid volume fraction may evolve to values greater than unity when growth leads to swelling of the multiphasic mixture.

Similarly, if solid-bound molecules are charged and their content evolves over time, the referential fixed charge density may also evolve with chemical reactions according to

$$c_r^F = c_0^F + \frac{1}{1 - \varphi_r^s}\sum_\sigma \frac{z^\sigma\rho_r^\sigma}{M^\sigma}\,, \tag{4.10.10}$$

where c_0^F is the referential fixed charge density specified by the multiphasic material parameter *fixed_charge_density* (Section 4.9.2). Thus, c_0^F may be used to account for the fixed charge density not contributed explicitly by solid-bound molecules.

A chemical reaction is properly balanced when

$$\sum_\alpha \nu^\alpha M^\alpha = 0\,, \tag{4.10.11}$$

where M^α is the molar mass of α. This constraint implies that the net gain in mass of products must be the same as the net loss in mass of reactants. However, this constraint is not verified in the code, allowing users to model chemical reactions with implicit constituents (constituents that are neither explicitly modeled as solutes nor as solid-bound molecules, for which ν^α and M^α are

not given). For example, a chemical reaction where cells consume glucose to form a protein from amino-acids building blocks may have the form

$$\text{cells} + \text{glucose} + \text{amino acids} \rightarrow \text{cells} + \text{protein} + \text{waste products}\,.$$

The user may opt to model only the glucose reactant and the protein product explicitly, while the presence of all other species in this reaction is implicit. In these types of analyses the user must beware of potential inconsistencies in the evolving mass of reactants and products since only some of those constituents are modeled explicitly. In particular, the evolution of φ_r^s as given in (4.10.9) can only account for the explicitly modeled solid-bound molecules. Furthermore, when some reactants and products are implicit, the value of the reaction molar volume $\overline{\mathcal{V}}$ calculated in the code becomes inaccurate and may produce unexpected results in the evaluation of the mixture mass balance relation in (4.10.6). Therefore, the user is given the option to override the value of $\overline{\mathcal{V}}$ calculated in the code. In particular, if the precise molar volumes of all the species in a reaction are not known, assuming that $\overline{\mathcal{V}} \approx 0$ is a reasonable choice equivalent to assuming that all the constituents have approximately the same density ρ_T^α, as may be deduced from (4.10.11).

Since the electroneutrality condition is enforced in multiphasic mixtures in FEBio, it follows that chemical reactions must not violate this condition. Enforcing electroneutrality in a chemical reaction is equivalent to satisfying

$$\sum_\alpha z^\alpha \nu^\alpha = 0\,. \tag{4.10.12}$$

This constraint is checked within the code and an error is generated when it is violated.

A constitutive relation must be provided for the molar production rate $\hat{\zeta}\left(\theta, \mathbf{F}, c^\alpha\right)$ of each chemical reaction.

4.10.2 General Specification for Chemical Reactions

The material type for a chemical reaction is "*reaction*". The <reaction> tag must appear inside the definition of a multiphasic mixture and the reaction is defined only for that mixture. Multiple chemical reactions may be defined in a given mixture. Each <reaction> tag must include a *type* attribute that identifies the constitutive relation for $\hat{\zeta}$.

The stoichiometric coefficients ν_R^α of the reactants and ν_P^α for the products must be specified in every reaction. Optionally, the net reaction molar volume $\overline{\mathcal{V}}$ may be specified explicitly to override the internal value calculated in the code. Therefore, the following parameters need to be defined in a chemical reaction:

<vR>	reactant stoichiometric coefficient ν_R^α	[ ]
<vP>	product stoichiometric coefficient ν_P^α	[ ]
<Vbar>	optional override value for $\overline{\mathcal{V}}$	[$\mathbf{L}^3$/**n**]

Each <vR> and <vP> tag must include either the *sol* attribute, which should reference a solute *id* from the <Solutes> description in the <Globals> section (Section 3.4.2), or the *sbm* attribute, which should reference a solid-bound molecule *id* from the <SolidBoundMolecules> description in the <Globals> section (Section 3.4.3). Only solutes and solid-bound molecules that have been included in the parent multiphasic mixture may be specified as reactants or products of a chemical reaction.

Additional parameters may be needed in the definition of a chemical reaction, depending on the specific form of the constitutive relation for the production rate.

4.10.3 Chemical Reaction Materials

4.10.3.1 Law of Mass Action for Forward Reactions

The material type for the Law of Mass Action for a forward reaction is *mass-action-forward*. The following parameters must be defined:

<forward_rate>	specific forward reaction rate k

For this type of reaction the constitutive relation for the molar production rate is given by

$$\hat{\zeta} = k \prod_{\alpha} (c^{\alpha})^{\nu_R^{\alpha}} \ .$$

The constitutive form of the specific forward reaction rate must be selected from the list of materials given in Section 4.10.4. The units of $\hat{\zeta}$ are [**n**/**L**^{3}·**t**] and those of c^{α} are [**n**/**L**^{3}].

Example:

Consider the forward reaction that produces solid copper sulfide from solid copper and solid sulfur,

$$\mathrm{Cu} + \mathrm{S} \rightarrow \mathrm{CuS}$$

All three species are modeled explicitly in the mixture as solid-bound molecules, with id's 1 (Cu), 2 (for S) and 3 (for CuS). The chemical reaction material is given by:

```
<reaction name="copper sulfide production" type="mass-action-forward">
  <vR sbm="1">1</vR>
  <vR sbm="2">1</vR>
  <vP sbm="3">1</vP>
  <forward_rate type="constant reaction rate">
    <k>1e-3</k>
  </forward_rate>
</reaction>
```

4.10.3.2 Law of Mass Action for Reversible Reactions

The material type for the Law of Mass Action for a reversible reaction is *mass-action-reversible*. The following parameters must be defined:

<forward_rate>	specific forward reaction rate k_F
<reverse_rate>	specific reverse reaction rate k_R

For this type of reaction the constitutive relation for the molar production rate is given by

$$\hat{\zeta} = \hat{\zeta}_F - \hat{\zeta}_R \,,$$

where

$$\hat{\zeta}_F = k_F \prod_\alpha (c^\alpha)^{\nu_R^\alpha}$$
$$\hat{\zeta}_R = k_R \prod_\alpha (c^\alpha)^{\nu_P^\alpha} \,.$$

The constitutive form of the specific forward and reverse reaction rates must be selected from the list of materials given in Section 4.10.4. The units of $\hat{\zeta}_F$ and $\hat{\zeta}_R$ are [**n**/**L**^{3}·**t**] and those of c^α are [**n**/**L**^{3}].

Example:

Consider the reversible dissociation of CaCl salt into Ca^{2+} and Cl^- in water,

$$CaCl_2 \rightleftharpoons Ca^{2+} + 2Cl^-$$

All three species are modeled explicitly in the mixture as solutes, with id's 1 (for $CaCl_2$), 2 (for Ca^{2+}) and 3 (for Cl^-). The chemical reaction material is given by:

```
<reaction name="CaCl2 dissociation" type="mass-action-reversible">
  <vR sol="1">1</vR>
  <vP sol="2">1</vP>
  <vP sol="3">2</vP>
  <forward_rate type="constant">
    <k>1.0</k>
  </forward_rate>
  <reverse_rate type="constant">
    <k>0.1</k>
  </reverse_rate>
</reaction>
```

4.10.3.3 Michaelis-Menten Reaction

The material type for the Michaelis-Menten reaction is *Michaelis-Menten*. The following parameters must be defined:

<forward_rate>	maximum rate at saturating substrate concentration $V_{\max}$	[**n**/**L**^{3}·**t**]
<Km>	substrate concentration when reaction rate is half of $V_{\max}$	[**n**/**L**^{3}]
<c0>	optional minimum substrate concentration to trigger reaction	[**n**/**L**^{3}]

The Michaelis-Menten reaction may be used to model enzyme kinetics where the enzyme $\mathcal{E}^e$ triggers the conversion of the substrate $\mathcal{E}^s$ into the product $\mathcal{E}^p$. The product molar supply is given by

$$\hat{c}^p = \begin{cases} \frac{V_{\max} c^s}{K_m + c^s} & c^s \geqslant c_0 \\ 0 & c^s < c_0 \end{cases},$$

where c^s is the substrate concentration. The default value of c_0 is 0. This relation may be derived, with some simplifying assumptions, by applying the law of mass action to the combination of two reactions,

$$\mathcal{E}^e + \mathcal{E}^s \rightleftharpoons \mathcal{E}^{es} \rightarrow \mathcal{E}^e + \mathcal{E}^p$$

Since the enzyme is not modeled explicitly in the Michaelis-Menten approximation to these two reactions, this reaction model is effectively equivalent to

$$\mathcal{E}^s \rightarrow \mathcal{E}^p.$$

Therefore, this reaction accepts only one reactant tag <vR> and one product tag <vP>. For consistency with the formulation of this reaction, the stoichiometric coefficients should be set to $\nu_R^s = \nu_P^p = 1$, so that $\hat{c}^p = \hat{\zeta}$.

The constitutive form of the specific forward reaction rate $V_{\max}$ must be selected from the list of materials given in Section 4.10.4.

Example:

```
<reaction name="enzyme kinetics" type="Michaelis-Menten">
  <Vbar>0</Vbar>
  <vR sol="1">1</vR>
  <vP sol="2">1</vP>
  <forward_rate type="constant">
    <k>1.0</k>
  </forward_rate>
  <Km>5.0</Km>
</reaction>
```

4.10.4 Specific Reaction Rate Materials

The following sections define specific materials that can be used to define the reaction rate of a chemical reaction.

4.10.4.1 Constant Reaction Rate

The material type for a constant specific reaction rate is *constant reaction rate*. The following parameter must be defined:

<k>	constant specific reaction rate k	[*units vary*]

Example:

```
<reaction name="enzyme kinetics" type="Michaelis-Menten">
  <Vbar>0</Vbar>
  <vR sol="1">1</vR>
  <vP sol="2">1</vP>
  <forward_rate type="constant reaction rate">
    <k>1.0</k>
  </forward_rate>
  <Km>5.0</Km>
</reaction>
```

4.10.4.2 Huiskes Reaction Rate

The material type for the Huiskes reaction rate is *Huiskes reaction rate*. The following parameters must be defined:

<B>	reaction rate per specific strain energy B	[*units vary*]
<psi0>	specific strain energy at homeostasis ψ_0	[**F**·**L**/**M**]

The Huiskes specific reaction rate has the form

$$k = \frac{B}{J - \varphi_r^s} \left(\frac{\Psi_r}{\rho_r^s} - \psi_0 \right) ,$$

where Ψ_r is the strain energy density of the solid (strain energy in current configuration per mixture volume in the reference configuration) and $\rho_r^s = \sum_\sigma \rho_r^\sigma$ is the referential apparent solid density (mass of solid in current configuration per mixture volume in reference configuration). The ratio Ψ_r/ρ_r^s is the specific strain energy (strain energy per mass of solid in the current configuration). The Huiskes specific reaction rate may assume positive and negative values; it reduces to zero at homeostasis, when $\Psi_r/\rho_r^s = \psi_0$.

Example:

To reproduce the interstitial solid remodeling theory proposed by Weinans et al. [57], consider the forward reaction

$$\text{cells} + \text{solutes} \rightarrow \text{cells} + \text{solid} ,$$

where cells convert solutes (e.g., nutrients) into synthesized solid when the specific strain energy exceeds the homeostatic value. If the cells and solutes are implicit in this reaction (e.g., if it is assumed that their concentrations change negligibly), the production rate of the solid may be given by $\hat{\zeta} = k$ using the law of mass action for a forward rection, where k has the form given above.

```
<reaction name="solid remodeling" type="mass-action-forward">
  <vP sbm="1">1</vP>
  <forward_rate type="Huiskes reaction rate">
    <B>1.0</B>
    <psi0>0.01</psi0>
  </forward_rate>
  <Km>5.0</Km>
</reaction>
```

4.11 Rigid Body

A rigid body can be defined using the rigid material model. The material type for a rigid body is "*rigid body*". The following parameters are defined:

<density>	Density of rigid body	[**M**/**L**^{3}]
<center_of_mass>	Position of the center of mass	[**L**]
<E>	Young's modulus	[**P**]
<v>	Poisson's ratio	[ ]

If the *center_of_mass* parameter is omitted, FEBio will calculate the center of mass automatically. In this case, a density *must* be specified. If the *center_of_mass* is defined the *density* parameter may be omitted. Omitting both will generate an error message.

The Young's modulus $E$and Poisson ratio v currently have no effect on the results. The only place where they are used is in the calculation of a material stiffness for some auto-penalty contact formulation. If you are using contact it is advised to enter sensible values. Otherwise these parameters may be omitted.

The degrees of freedom of a rigid body are initially unconstrained[3]. This implies that a rigid body is free to move in all three directions and rotate about any of the coordinate axes. To constrain a rigid body degree of freedom you may use the *Boundary* section (Section 3.11.1) or *Constraints* sections (Section 3.14.1).

Example:

```
<material id="1" type="rigid body">
  <density>1.0</density>
  <center_of_mass>0,0,0</center_of_mass>
</material>
```

[3]This is different from previous versions of FEBio where rigid bodies were initially fully constrained.

4.12 Active Contraction

Active contraction materials may be used to impose a (typically) contractile stress within a solid material, by incorporating the contraction material within a solid mixture. The total stress in the solid mixture is simply $\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^a$, where $\boldsymbol{\sigma}^s$ is the solid stress (due to strain and strain history), and $\boldsymbol{\sigma}^a$ is the active contractile stress. The calculation of the contractile stress is the same, wether the solid mixture consists of uncoupled or compressible materials.

4.12.1 Contraction in Mixtures of Uncoupled Materials

When the solid mixture consists of uncoupled materials, the active contraction material should be selected from the list below.

4.12.1.1 Uncoupled Prescribed Uniaxial Active Contraction

The material type for prescribed active contraction along a single direction (or fiber) in an uncoupled solid mixture is "*uncoupled prescribed uniaxial active contraction*". This material must be combined with a stable uncoupled material that acts as a passive matrix, using a "*uncoupled solid mixture*" container as described in Section 4.1.2.15. The following material parameters need to be defined:

<T0>	T_0, representing the prescribed stress	[**P**]

In the reference configuration, the fiber is oriented along the unit vector $\mathbf{e}_1$, where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are orthonormal basis vectors representing the local element coordinate system when specified (Section 4.1.1), or else the global Cartesian coordinate system. The active stress $\boldsymbol{\sigma}^a$ for this material is given by

$$\boldsymbol{\sigma}^a = J^{-1} T_0 \mathbf{n} \otimes \mathbf{n} \,,$$

where $\mathbf{n} = \mathbf{F} \cdot \mathbf{n}_r$ is the stretched fiber orientation in the current (deformed) configuration.

Example:

Uniaxial contraction along $\mathbf{e}_1$, in a mixture containing a Mooney-Rivlin solid.

```
<material id="1" type="uncoupled solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>1.0</c1>
    <c2>0</c2>
    <k>1000</k>
  </solid>
  <solid type="prescribed uniaxial active contraction uncoupled">
    <T0 lc="2">1</T0>
    <mat_axis type="angles">
      <theta>0</theta>
      <phi>90</phi>
    </mat_axis>
  </solid>
</material>
```

4.12.1.2 Uncoupled Prescribed Transversely Isotropic Active Contraction

The material type for prescribed isotropic active contraction in a plane transverse to a given direction (or fiber), in an uncoupled solid mixture, is "*prescribed trans iso active contraction uncoupled*". This material must be combined with a stable uncoupled material that acts as a passive matrix, using a "*uncoupled solid mixture*" container as described in Section 4.1.2.15. The following material parameters need to be defined:

<T0>	T_0, representing the prescribed stress	[**P**]

In the reference configuration, the fiber is oriented along the unit vector $\mathbf{e}_1$, where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are orthonormal basis vectors representing the local element coordinate system when specified

(Section 4.1.1), or else the global Cartesian coordinate system. The active stress $\boldsymbol{\sigma}^a$ for this material is given by

$$\boldsymbol{\sigma}^a = J^{-1} T_0 \left(\mathbf{B} - \mathbf{n} \otimes \mathbf{n} \right) ,$$

where $\mathbf{n} = \mathbf{F} \cdot \mathbf{e}_1$ is the stretched fiber orientation in the current (deformed) configuration and $\mathbf{B} = \mathbf{F} \cdot \mathbf{F}^T$ is the left Cauchy-Green tensor.

Example:
Isotropic contraction in plane transverse to $\mathbf{e}_1$, in a mixture containing a Mooney-Rivlin solid.

```
<material id="1" type="uncoupled solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>1.0</c1>
    <c2>0</c2>
    <k>1000</k>
  </solid>
  <solid type="prescribed trans iso active contraction uncoupled">
    <T0 lc="2">1</T0>
    <mat_axis type="angles">
      <theta>0</theta>
      <phi>90</phi>
    </mat_axis>
  </solid>
</material>
```

4.12.1.3 Uncoupled Prescribed Isotropic Active Contraction

The material type for prescribed isotropic active contraction, in an uncoupled solid mixture, is "*prescribed isotropic active contraction uncoupled*". This material must be combined with a stable uncoupled material that acts as a passive matrix, using a "*uncoupled solid mixture*" container as described in Section 4.1.2.15. The following material parameters need to be defined:

<T0>	T_0, representing the prescribed stress	[**P**]

The active stress $\boldsymbol{\sigma}^a$ for this material is given by

$$\boldsymbol{\sigma}^a = J^{-1} T_0 \mathbf{B} \, .$$

Note: If the solid material in the mixture is (nearly) incompressible, this isotropic contraction will cause no change in the deformation.

Example:
Isotropic contraction in a mixture containing a Mooney-Rivlin solid.

```
<material id="1" type="uncoupled solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>1.0</c1>
    <c2>0</c2>
    <k>5.0</k>
```

```
  </solid>
  <solid type="prescribed isotropic active contraction uncoupled">
    <T0 lc="2">1</T0>
  </solid>
</material>
```

4.12.1.4 Prescribed Fiber Stress

An active fiber stress, based on a Hill formulation, can be added via the material "*uncoupled active fiber stress*". This material must be combined with a stable compressible material that acts as a passive matrix, using a "*uncoupled solid mixture*" container as described in Section 4.1.2.15. The stress is given by,

$$\boldsymbol{\sigma}^a = J^{-1} T\left(\tilde{\lambda}\right) \mathrm{dev}\mathbf{A}.$$

Here, $\mathbf{A} = \mathbf{a} \otimes \mathbf{a}$,with **a** the unit vector describing the fiber direction in the spatial frame, $\tilde{\lambda}$is the deviatoric fiber stretch, *J* is the jacobian of the deformation, and

$$T\left(\tilde{\lambda}\right) = s_{max} a\left(t\right) s_{TL}\left(\tilde{\lambda}\right) s_{TV}\left(\dot{\tilde{\lambda}}\right)$$

The parameters are defined below.

smax	scale factor for defining maximum stress	[**P**]
a	activation level	
stl	Function defining the stress-stretch relatioship for the material	
stv	Function defining the stress-stretch rate relatioship for the material.	

The parameters$s_{TL}$and $s_{TV}$are functions that need to be defined in place. There are currently two ways of defining these functions, either via a mathematical expression or a list of sample points. An example is given below. If these parametes are omitted, they are replaced by the constant 1 in the equation for the stress above.

Example:

An example defining the stl parameter via a mathematical expression.

```
<material id="1" type="uncoupled solid mixture">
  <k>100.0</k>
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>1.0</c1>
    <c2>0</c2>
  </solid>
  <solid type="uncoupled active fiber stress">
    <smax>1.5</smax>
    <a lc="1">0.1</a>
    <stl type="math">
      <math>(l-1)^2</math>
    <stl>
  </solid>
</material>
```

An example defining the stl parameter via a point list.

```
<material id="1" type="uncoupled solid mixture">
  <k>100.0</k>
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="Mooney-Rivlin">
    <c1>1.0</c1>
    <c2>0</c2>
  </solid>
  <solid type="uncoupled active fiber stress">
    <smax>1.5</smax>
    <a lc="1">0.1</a>
    <stl type="point">
      <interpolate>linear</interpolate>
      <points>
        <pt>0,0</pt>
        <pt>1,0</pt>
        <pt>2,1</pt>
      </points>
    <stl>
  </solid>
</material>
```

4.12.2 Contraction in Mixtures of Compressible Materials

When the solid mixture consists of compressible materials, the active contraction material should be selected from the list below.

4.12.2.1 Prescribed Uniaxial Active Contraction

The material type for prescribed active contraction along a single direction (or fiber) in a solid mixture of compressible materials is "*prescribed uniaxial active contraction*". This material must be combined with a stable compressible material that acts as a passive matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<T0>	T_0, representing the prescribed stress	[**P**]

In the reference configuration, the fiber is oriented along the unit vector $\mathbf{e}_1$, where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are orthonormal basis vectors representing the local element coordinate system when specified (Section 4.1.1), or else the global Cartesian coordinate system. The active stress $\boldsymbol{\sigma}^a$ for this material is given by

$$\boldsymbol{\sigma}^a = J^{-1} T_0 \mathbf{n} \otimes \mathbf{n} \,,$$

where $\mathbf{n} = \mathbf{F} \cdot \mathbf{e}_1$ is the stretched fiber orientation in the current (deformed) configuration.

Example:

Uniaxial contraction along $\mathbf{e}_1$, in a mixture containing a neo-Hookean solid.

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1.0</E>
    <v>0.3</v>
  </solid>
  <solid type="prescribed uniaxial active contraction">
    <T0 lc="2">1</T0>
    <mat_axis type="angles">
      <theta>0</theta>
      <phi>90</phi>
    </mat_axis>
  </solid>
</material>
```

4.12.2.2 Prescribed Transversely Isotropic Active Contraction

The material type for prescribed isotropic active contraction in a plane transverse to a given direction (or fiber), in a solid mixture of compressible materials, is "*prescribed trans iso active contraction*". This material must be combined with a stable compressible material that acts as a passive matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<T0>	T_0, representing the prescribed stress	[**P**]

In the reference configuration, the fiber is oriented along the unit vector $\mathbf{e}_1$, where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are orthonormal basis vectors representing the local element coordinate system when specified (Section 4.1.1), or else the global Cartesian coordinate system. The active stress $\boldsymbol{\sigma}^a$ for this material is given by

$$\boldsymbol{\sigma}^a = J^{-1} T_0 \left(\mathbf{B} - \mathbf{n} \otimes \mathbf{n} \right) ,$$

where $\mathbf{n} = \mathbf{F} \cdot \mathbf{e}_1$ is the stretched fiber orientation in the current (deformed) configuration and $\mathbf{B} = \mathbf{F} \cdot \mathbf{F}^T$ is the left Cauchy-Green tensor.

Example:

Isotropic contraction in plane transverse to $\mathbf{e}_1$, in a mixture containing a neo-Hookean solid.

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1.0</E>
    <v>0.3</v>
  </solid>
  <solid type="prescribed trans iso active contraction">
    <T0 lc="2">1</T0>
    <mat_axis type="angles">
      <theta>0</theta>
      <phi>90</phi>
    </mat_axis>
  </solid>
</material>
```

4.12.2.3 Prescribed Isotropic Active Contraction

The material type for prescribed isotropic active contraction, in a solid mixture of compressible materials, is "*prescribed isotropic active contraction*". This material must be combined with a stable compressible material that acts as a passive matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The following material parameters need to be defined:

<T0>	T_0, representing the prescribed stress	[**P**]

The active stress $\boldsymbol{\sigma}^a$ for this material is given by

$$\boldsymbol{\sigma}^a = J^{-1} T_0 \mathbf{B} \, .$$

Example:

Isotropic contraction in a mixture containing a neo-Hookean solid.

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1.0</E>
    <v>0</v>
  </solid>
  <solid type="prescribed isotropic active contraction">
    <T0 lc="2">1</T0>
  </solid>
</material>
```

4.12.2.4 Prescribed Fiber Stress

An active fiber stress, based on a Hill formulation, can be added via the material "*active fiber stress*". This material must be combined with a stable compressible material that acts as a passive matrix, using a "*solid mixture*" container as described in Section 4.1.3.23. The stress is given by,

$$\boldsymbol{\sigma}^a = J^{-1} T(\lambda)\, \mathbf{A}.$$

Here, $\mathbf{A} = \mathbf{a} \otimes \mathbf{a}$,with **a** the unit vector describing the fiber direction in the spatial frame, $\lambda$is the fiber stretch, *J* is the jacobian of the deformation, and

$$T(\lambda) = s_{max} a(t)\, s_{TL}(\lambda)\, s_{TV}\left(\dot{\lambda}\right)$$

The parameters are defined below.

smax	scale factor for defining maximum stress	[**P**]
a	activation level	
stl	Function defining the stress-stretch relatioship for the material	
stv	Function defining the stress-stretch rate relatioship for the material.	

The parameters$s_{TL}$and $s_{TV}$are functions that need to be defined in place. There are currently two ways of defining these functions, either via a mathematical expression or a list of sample points. An example is given below. If these parametes are omitted, they are replaced by the constant 1 in the equation for the stress above.

Example:

An example defining the stl parameter via a mathematical expression.

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1.0</E>
    <v>0</v>
  </solid>
  <solid type="active fiber stress">
    <smax>150</smax>
    <a lc="1">0.1</a>
    <stl type="math">
      <math>(l-1)^2</math>
    <stl>
  </solid>
</material>
```

An example defining the stl parameter via a point list.

```
<material id="1" type="solid mixture">
  <mat_axis type="local">0,0,0</mat_axis>
  <solid type="neo-Hookean">
    <E>1.0</E>
    <v>0</v>
```

```
    </solid>
    <solid type="active fiber stress">
      <smax>150</smax>
      <a lc="1">0.1</a>
      <stl type="point">
        <interpolate>linear</interpolate>
        <points>
          <pt>0,0</pt>
          <pt>1,0</pt>
          <pt>2,1</pt>
        </points>
      <stl>
    </solid>
  </material>
```

4.13 Viscous Fluids

Fluid mechanics analyses may be used to examine fluid flow over fixed domains. Fluid-structure interactions (FSI) may be used to examine fluid flow over deforming domains. FEBio's fluid and fluid-FSI modules treat the fluid as isothermal (constant and uniform temperature) and compressible; incompressible flow is simulated by prescribing a physically realistic bulk modulus K to model the fluid's elastic compressibility (for example, $K = 2.2$ GPa for water at room temperature). The Cauchy stress $\boldsymbol{\sigma}^f$ in a fluid is given by

$$\boldsymbol{\sigma}^f = -p\mathbf{I} + \boldsymbol{\tau}\,, \tag{4.13.1}$$

where p is the fluid pressure arising from the elastic response and $\boldsymbol{\tau}$ is the viscous stress resulting from the fluid viscosity and its rate of deformation. The fluid pressure is evaluated from

$$p = K\left(1 - J^f\right) = -K\,e^f\,, \tag{4.13.2}$$

whre J^f is the fluid volume ratio and $e^f = J^f - 1$ is the dilatation (the relative change in volume). The fluid density ρ^f varies with J^f according to

$$\rho^f = \frac{\rho_r^f}{J^f}\,, \tag{4.13.3}$$

where ρ_r^f is the fluid density in the reference configuration (when the pressure p is zero). The dependence of $\boldsymbol{\tau}$ on the fluid rate of deformation tensor $\mathbf{D}^f = \frac{1}{2}\left(\operatorname{grad}\mathbf{v}^f + \operatorname{grad}^T\mathbf{v}^f\right)$, where $\mathbf{v}^f$ =fluid velocity, is given by a constitutive model which may be chosen from the list provided in Section 4.13.2. Though Newtonian and non-Newtonian fluids may be analyzed in this framework, all fluids are purely viscous (no viscoelasticity is included in this formulation). Setting the viscosity to zero is allowable, for the purpose of analyzing inviscid flow. The user is referred to the *FEBio Theory Manual* for a general description of this isothermal compressible viscous flow framework.

For fluid analyses, which are performed over a fixed mesh, FEBio solves for the components of the fluid velocity $\mathbf{v}^f$ and fluid dilatation e^f at each node. In contrast, fluid-FSI analyses are performed over deforming meshes and FEBio treats fluid-FSI domains as a mixture of a viscous fluid f and a massless, frictionless porous solid s. Thus, the fluid encounters zero resistance as it flows

through the deforming mesh (porous solid). The solid constituent of a fluid-FSI domain regularizes the mesh deformation; it is a hyperelastic solid whose constitutive relation is selected by the user; the recommended choice is the compressible neo-Hookean solid defined in Section 4.1.3.17, with $\nu = 0$ and E set to a very small (but non-zero) value. For fluid-FSI analyses, FEBio solves for the solid displacement $\mathbf{u}$, the fluid velocity $\mathbf{w}$ relative to the mesh, and the fluid dilatation e^f. The fluid velocity is then calculated as

$$\mathbf{v}^f = \mathbf{v}^s + \mathbf{w}\,, \tag{4.13.4}$$

where $\mathbf{v}^s$ is the mesh velocity (the material time derivative of the solid displacement $\mathbf{u}$). Since the mesh is fixed in a standard fluid analysis, $\mathbf{v}^s = \mathbf{0}$ and $\mathbf{v}^f = \mathbf{w}$ in that case. Therefore, we use $\mathbf{w}$ to refer to the fluid velocity degrees of freedom for fluid and fluid-FSI analyses. For both types of analyses, the no-slip condition for viscous fluids flowing along a boundary is satisfied by setting $\mathbf{w} = \mathbf{0}$ on that boundary.

On any fluid boundary, the outward surface normal may be denoted by $\mathbf{n}$ and the traction vector on the fluid is given by $\mathbf{t}^f = \boldsymbol{\sigma}^f \cdot \mathbf{n} = -p\,\mathbf{n} + \mathbf{t}^\tau$, where $\mathbf{t}^\tau = \boldsymbol{\tau} \cdot \mathbf{n}$ is the viscous traction. Essential (Dirichlet) boundary conditions may be prescribed on $\mathbf{w}$ and e^f, while natural (Neumann) boundary conditions may be prescribed on $\mathbf{t}^\tau$ and w_n. The appearance of velocity in both essential and natural boundary conditions may seem surprising at first. To better understand the nature of these boundary conditions, it is convenient to separate the velocity into its normal and tangential components, $\mathbf{w} = w_n\mathbf{n} + \mathbf{w}_t$, where $\mathbf{w}_t = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \mathbf{w}$. In particular, for inviscid flow, the viscous stress $\boldsymbol{\tau}$ and its corresponding traction $\mathbf{t}^\tau$ are both zero, leaving w_n as the sole natural boundary condition; similarly, e^f becomes the only essential boundary condition in such flows, since $\mathbf{w}_t$ is unknown *a priori* on a frictionless boundary and must be obtained from the solution of the analysis.

In general, prescribing e^f is equivalent to prescribing the elastic fluid pressure, since p is only a function of e^f. On a boundary where no conditions are prescribed explicitly, we conclude that $w_n = 0$ and $\mathbf{t}^\tau = \mathbf{0}$, which represents a frictionless wall. Conversely, it is possible to prescribe w_n and $\mathbf{t}^\tau$ on a boundary to produce a desired inflow or outflow while simultaneously stabilizing the flow conditions by prescribing a suitable viscous traction. Prescribing essential boundary conditions $\mathbf{w}_t$ and e^f determines the tangential velocity on a boundary as well as the elastic fluid pressure p, leaving the option to also prescribe the normal component of the viscous traction, $t_n^\tau = \mathbf{t}^\tau \cdot \mathbf{n}$, to completely determine the normal traction $t_n^f = \mathbf{t}^f \cdot \mathbf{n}$ (or else t_n^τ naturally equals zero). Mixed boundary conditions represent common physical features: Prescribing w_n and $\mathbf{w}_t$ completely determines the velocity $\mathbf{w}$ on a boundary; prescribing $\mathbf{t}^\tau$ and e completely determines the traction $\mathbf{t}^f = \boldsymbol{\sigma}^f \cdot \mathbf{n}$ on a boundary. Note that w_n and e^f are mutually exclusive boundary conditions, and the same holds for $\mathbf{w}_t$ and the tangential component of the viscous traction, $\mathbf{t}_t^\tau = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \mathbf{t}^\tau$.

For viscous fluids, the no-slip boundary condition at an impermeable wall is enforced by setting $\mathbf{w}_t = \mathbf{0}$, whereas the wall impermeability condition implies $w_n = 0$. Therefore, these conditions may be combined by prescribing wx, wy and wz components of $\mathbf{w}$ to zero. FEBio offers a range of options for conveniently prescribing natural and mixed conditions on boundary surfaces in fluid analyses (Section 3.12.2).

4.13.1 General Specification of Fluid Materials

The material type for a fluid material is *"fluid"*. The following parameters must be defined:

<density>	Fluid referential density ρ_r	[**M**/**L**^{3}]
<k>	Bulk modulus K	[**P**]
<viscous>	Specification of viscous model for $\boldsymbol{\tau}$	

The <viscous> tag encloses a description of the viscous stress constitutive relation and associated material properties, as may be selected from the list provided in Section 4.13.2. The parameters <density> and <k> must be greater than 0. These parameters are always required.

Example:

```
<material id="1" name="Water" type="fluid">
<density>1</density>
<k>2.2e+09</k>
<viscous type="Newtonian fluid">
<mu>0.001</mu>
<kappa>0</kappa>
</viscous>
</material>
```

4.13.2 Viscous Fluid Materials

Viscous fluid materials provide a constitutive relation for the dependence of the viscous stress $\boldsymbol{\tau}$ on the rate of deformation tensor $\mathbf{D}^f$ of a fluid.

4.13.2.1 Newtonian Fluid

The material type for a Newtonian fluid is "*Newtonian fluid*". The following material parameters must be defined:

<mu>	shear viscosity μ	[**P**·**t**]
<kappa>	bulk viscosity κ	[**P**·**t**]

The viscous shear stress for this material model is

$$\boldsymbol{\tau} = \left(\kappa - \frac{2}{3}\mu\right)(\operatorname{tr}\mathbf{D})\,\mathbf{I} + 2\mu\mathbf{D}$$

Stokes' condition is a constitutive assumption that sets $\operatorname{tr}\boldsymbol{\tau} = 0$, implying that $\kappa = 0$. This assumption is only valid for some fluids (e.g., monoatomic gas [46]). Users may use or ignore this assumption by selecting an appropriate value for κ.

Example:

```
<viscous type="Newtonian fluid">
<mu>0.001</mu>
<kappa>0</kappa>
</viscous>
```

4.13.2.2 Carreau Model

The material type for a Carreau model [22] is "*Carreau*". The following material parameters must be defined:

<mu0>	shear viscosity at zero shear rate, μ_0	[**P**·**t**]
<mui>	shear viscosity at infinite shear rate, μ_∞	[**P**·**t**]
<lambda>	time constant	[**t**]
<n>	power-law exponent	

The viscous shear stress for this material model is

$$\boldsymbol{\tau} = 2\mu\mathbf{D}$$

where

$$\mu = \mu_\infty + (\mu_0 - \mu_\infty)\left(1 + (\lambda\dot{\gamma})^2\right)^{(n-1)/2}$$

Here, $\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}$ is the engineering shear rate.

Example:

```
<viscous type="Carreau">
<mu0>0.056</mu0>
<mui>0.0035</mui>
<lambda>3.3</lambda>
<n>0.36</n>
</viscous>
```

4.13.2.3 Carreau-Yasuda Model

The material type for a Carreau-Yasuda model [22] is "*Carreau-Yasuda*". The following material parameters must be defined:

<mu0>	shear viscosity at zero shear rate, μ_0	[**P**·**t**]
<mui>	shear viscosity at infinite shear rate, μ_∞	[**P**·**t**]
<lambda>	time constant	[**t**]
<n>	power-law exponent	
<a>	power-law exponent divider	

The viscous shear stress for this material model is

$$\boldsymbol{\tau} = 2\mu\mathbf{D}$$

where

$$\mu = \mu_\infty + (\mu_0 - \mu_\infty)\left(1 + (\lambda\dot{\gamma})^a\right)^{(n-1)/a}$$

Here, $\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}$ is the engineering shear rate.

Example:

```
<viscous type="Carreau-Yasuda">
<mu0>0.056</mu0>
<mui>0.0035</mui>
<lambda>1.9</lambda>
<n>0.22</n>
<a>1.25</a>
</viscous>
```

4.13.2.4 Powell-Eyring Model

The material type for a Powell-Eyring model [22] is "*Powell-Eyring*". The following material parameters must be defined:

<mu0>	shear viscosity at zero shear rate, μ_0	[**P**·**t**]
<mui>	shear viscosity at infinite shear rate, μ_∞	[**P**·**t**]
<lambda>	time constant	[**t**]

The viscous shear stress for this material model is

$$\boldsymbol{\tau} = 2\mu\mathbf{D}$$

where

$$\mu = \mu_\infty + (\mu_0 - \mu_\infty)\,\frac{\sinh^{-1}\lambda\dot{\gamma}}{\lambda\dot{\gamma}}$$

Here, $\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}$ is the engineering shear rate.

Example:

```
<viscous type="Powell-Eyring">
<mu0>0.056</mu0>
<mui>0.0035</mui>
<lambda>5.4</lambda>
</viscous>
```

4.13.2.5 Cross Model

The material type for a Cross model [22] is "*Cross*". The following material parameters must be defined:

<mu0>	shear viscosity at zero shear rate, μ_0	[**P**·**t**]
<mui>	shear viscosity at infinite shear rate, μ_∞	[**P**·**t**]
<lambda>	time constant	[**t**]
<m>	exponent	

The viscous shear stress for this material model is

$$\boldsymbol{\tau} = 2\mu\mathbf{D}$$

where

$$\mu = \mu_\infty + (\mu_0 - \mu_\infty)\,\frac{1}{1 + (\lambda\dot{\gamma})^m}$$

Here, $\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}$ is the engineering shear rate.

Example:

```
<viscous type="Cross">
<mu0>0.056</mu0>
<mui>0.0035</mui>
<lambda>1.0</lambda>
<m>1.0</m>
</viscous>
```

4.13.3 General Specification of Fluid-FSI Materials

The material type for a fluid-FSI material is *"fluid-FSI"*. This type of material is used for fluid flow through a deforming mesh. The material is treated as a special case of fluid-solid mixture, with the solid material used to regularize the mesh deformation. The following parameters must be defined:

<fluid>	Specification of fluid model	
<solid>	Specification of elastic solid model for mesh deformation	

The <fluid> tag encloses a description of the fluid, as given in Section 4.13.1. The <solid> tag encloses a description of the solid, which should be modeled as a compressible elastic solid, as given in Section 4.1.3. The recommended choice is the compressible neo-Hookean solid defined in Section 4.1.3.17, with $\nu = 0$ and E set to a very small (but non-zero) value.

Example:

```
<material id="1" name="Fluid-FSI domain" type="fluid-FSI">
<fluid type="fluid">
<density>1000</density>
<k>2.2e9</k>
<viscous type="Newtonian fluid">
<mu>0.001</mu>
<kappa>0</kappa>
</viscous>
</fluid>
<solid type="neo-Hookean">
<density>0</density>
<E>1e-9</E>
<v>0</v>
</solid>
</material>
```

The value of <density> in the <solid> material is internally set to zero regardless of the user-defined value, since the deforming mesh should not be subjected to inertial forces.

4.14 Prestrain material

In FEBio a prestrain can be defined for most materials that allows the user to prestrain or prestress the model before loading is applied. This is useful for modeling biologically tissues that exhibit residual strain, or whose initial state cannot assumed to be stress-free (e.g. arteries from in-vivo image data.)

If you use this feature in your published research, please cite the corresponding paper that details the theoretical framework and the implementation in FEBio [41].

4.14.1 Introduction

In the modeling of biological tissues there are various reasons why the model needs to start from a prestressed configuration. For example, the biological tissue may exhibit residual stress

or in situ stress. Or the geometry is taken from in vivo data and is subjected to loads in the reference configuration. In these cases, the reference configuration cannot be considered stress-free and this so-called prestress must somehow be accounted for. In large strain analysis, stresses are usually not additive and in addition, it must somehow be ensured that these prestresses are in equilibrium in the reference configuration. In general, this makes prestressing the reference configuration challenging in large strain analyses.

Progress can be made by assuming that the material is hyperelastic and that a prestrain can be found that defines the prestress via the hyperelastic constitutive formulation. Usually this prestrain is characterized by a second-order tensor, termed the prestrain gradient and here denoted by $\boldsymbol{F}_p$. The interpretation of this tensor is that its inverse, applied to a small neighborhood of a point in the reference configuration, would render this neighborhood stress-free. The total elastic response of the material is then defined via the elastic deformation gradient.

$$\boldsymbol{F_e} = \boldsymbol{F} \cdot \boldsymbol{F_p} \tag{4.14.1}$$

Here, $\boldsymbol{F}$is the deformation gradient that is the result of subsequent loading of the reference configuration. Finally, the Cauchy stress and spatial elasticity tangent are given by

$$\boldsymbol{\sigma} = \boldsymbol{\mathcal{F}}\left(\boldsymbol{F_e}\right), \boldsymbol{c} = \boldsymbol{\mathcal{G}}\left(\boldsymbol{F_e}\right) \tag{4.14.2}$$

Here, $\boldsymbol{\mathcal{F}}$ and $\boldsymbol{G}$ are the same response functions from the "natural" material, i.e. the response of the material that starts from a stress-free configuration.

It must be noted that although $\boldsymbol{F}_p$ is termed the prestrain gradient, in general it will not be the derivative of a deformation map. Consequently, a global stress-free reference configuration may not exist and the mapping of a neighborhood in the reference configuration to a stress-free state can at best be defined only locally.

In addition, it must also be recognized that the prestrain gradient is not unique. Due to the requirements of objectivity in the presence of material symmetries, the prestrain gradients $\boldsymbol{F}_p$ and $\boldsymbol{F'}_p = \boldsymbol{F_p}\boldsymbol{Q}$, where $\boldsymbol{Q}$ is any orthogonal tensor, must result in the same material response. This implies that the prestrain can only be dependent on the right stretch tensor $\boldsymbol{V_p}$. However, in general even the right-stretch tensor cannot be defined uniquely. For instance, an isotropic material would only depend on the eigenvalues of this tensor and thus any tensor of the form $\boldsymbol{RDR^T}$, where $\boldsymbol{R}$ is any orthogonal tensor and $\boldsymbol{D}$ is a diagonal tensor with the three eigenvalues of $\boldsymbol{V_p}$on its diagonal, would render the same material response. In the presence of material symmetries, the situation is similar although $\boldsymbol{R}$ will only be part of the symmetry group.

Despite the fact that $\boldsymbol{F}_p$ is not unique, it is far from arbitrary. The most important restriction is that the resulting prestress field $\boldsymbol{\sigma}_p$must be in equilibrium with the prestressed reference configuration. In other words it must hold that

$$div\boldsymbol{\sigma}_p = \boldsymbol{0} \tag{4.14.3}$$

in the interior of the reference domain (in the absence of body forces) and that on the free boundaries of the domain

$$\boldsymbol{\sigma}_p \cdot \boldsymbol{n} = 0 \tag{4.14.4}$$

In a finite element simulation, when these conditions are not satisfied, the mesh will distort and a new reference state is obtained as well as an altered prestrain field. We will denote the deformation gradient between the original (incompatible) reference configuration and prestressed reference configuration by $\boldsymbol{F}_c$. When the mesh distorts the effectively applied prestrain field is

also altered. In general, this is not desired and a correction to the prestrain field is necessary that either eliminates the distortion or finds a new reference geometry in which the desired prestrain field is supported.

The prestrain framework as currently implemented assumes that the total effective prestrain that is compatible with the possibly altered prestressed reference configuration is given by the following multiplicative decomposition.

$$\boldsymbol{F}_p = \boldsymbol{F}_c \cdot \hat{\boldsymbol{F}}_p \tag{4.14.5}$$

Both the prestrain gradient and the distortion are in general unknown. The framework implements an iterative algorithm that updates $\boldsymbol{F}_c$ and $\hat{\boldsymbol{F}}_p$ until an effective prestrain gradient is found that is compatible with the possibly distorted reference configuration. Without loss of generality the framework assumes that the altered prestrain gradient $\hat{\boldsymbol{F}}_p$is itself given by the multiplicative decomposition

$$\hat{\boldsymbol{F}}_p = \boldsymbol{G} \cdot \boldsymbol{F}_0 \tag{4.14.6}$$

where $\mathbf{F}_0$ is an initial guess for the prestrain gradient and $\mathbf{G}$ is a correction factor. The algorithm starts by initializing $\mathbf{F}_0$ to a user-defined value and $\mathbf{G}$ to the identity. This initial value can be specified in a variety of ways and the code that generates this initial guess is called the prestrain generator. The framework provides several prestrain generators and users can easily add new ones. Then, a forward analysis is executed keeping $\hat{\mathbf{F}}_p$fixed. Unless the initial guess was compatible with the reference configuration, the mesh will distort. This distortion will define the new value for $\mathbf{G}$ which can be calculated directly from the nodal displacements in the usual manner. Next, the framework will update using a user-defined update rule. How $\mathbf{G}$ is updated depends on the particular application and the framework expects the user do provide the desired update rule. The current implementation provides two particular update rules: one to eliminate the distortion and one to enforce a particular form of the prestrain gradient. See section ?? on how to use these update rules. In addition, users can easily implement new update rules. After this update, a new forward analysis is executed. This process is repeated until $\mathbf{G}$ converges.

4.14.2 The Prestrain Material

Prestrain can be applied by defining the prestrain material. This material acts as a wrapper to the underlying elastic constitutive model. There are two flavors of this material, one for coupled materials and one for uncoupled. In either case, the material defines two properties. The *elastic* property defines the elastic constitutive model. Any of the materials in FEBio could be used, however, the prestrain material has only been validated for hyperelastic materials. The second property, called *prestrain*, defines the prestrain generator. This property defines how the initial prestrain gradient is calculated. Currently, it can be defined as a full second order matrix or as a fiber stretch. The prestrain data can be defined at the material level or at the element level.

The *prestrain* property defines the way that the initial prestrain gradient tensor is calculated. An algorithm that calculates the initial prestrain based on user input is here referred to as a prestrain generator. The type attribute is used to create a specific instance of a prestrain generator. Currently, the following generators are available.

4.14.2.1 prestrain gradient

The *prestrain gradient* generator defines the full prestrain gradient matrix either for the entire material or for each element separately. It has one parameter, namely the prestrain gradient for the entire material.

parameter	description
F0	3x3 initial prestrain gradient matrix

Example:

```
<material id="1" type="prestrain elastic">
  <elastic type="neo-Hookean">
    <E>1.0</E>
    <v>0.3</v>
  </elastic>
  <prestrain type="prestrain gradient">
    <F0>1,0,0,0,1,0,0,0,1</F0>
  </prestrain>
</material>
```

4.14.2.2 in-situ stretch

The *in-situ stretch* generator option calculates a prestrain gradient based on a fiber stretch and the fiber vector defined by the parent material.

parameter	description	initial values
stretch	initial fiber stretch	1.0
isochoric	use the isochoric prestrain generator option	1

This option generates one of the following prestrain gradients, depending on the isochoric option.

$$\hat{\mathbf{F}}_{p,iso} = \mathbf{Q}\begin{bmatrix} \lambda & & \\ & \lambda^{-1/2} & \\ & & \lambda^{-1/2} \end{bmatrix}\mathbf{Q}^T, \qquad \hat{\mathbf{F}}_{p,uni} = \mathbf{Q}\begin{bmatrix} \lambda & & \\ & 1 & \\ & & 1 \end{bmatrix}\mathbf{Q}^T \tag{4.14.7}$$

If the *isochoric* option is set to 1, then $\hat{\mathbf{F}}_{p,iso}$is used. Otherwise, $\hat{\mathbf{F}}_{p,uni}$is used.

Example:

```
<material id="1" type="prestrain elastic">
  <elastic type="neo-Hookean">
    <E>1.0</E>
    <v>0.3</v>
  </elastic>
  <prestrain type="in-situ stretch">
    <stretch lc="1">1.05</stretch>
    <isochoric>1</isochoric>
  </prestrain>
</material>
```

Chapter 5

Restart Input file

5.1 Introduction

Users can request FEBio to output a binary dump file. This dump file can be used to restart the analysis from the time point saved in the dump file. The user can restart the analysis either directly from this binary dump file or via a restart input file, which is described in this chapter. See section 2.8.3 for more information on how to use the restart feature.

This chapter describes the format of the restart input file. This file is used to redefine some parameters when restarting a previously terminated run and can also be used to extend the analysis. The structure is very similar to the FEBio input file and also uses XML formatting. Since the file uses XML, the first line must be the XML header:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
```

The next line contains the root element of the restart file, and has to be:

```
<febio_restart version="2.0">
```

The restart file is composed of the following sections. These sections are sub-elements of the *febio_restart* root element.

Archive define the binary dump file used for restarting.

Control redefine some control parameters.

LoadData redefine or add some loadcurves.

Step add an analysis step.

All sections are optional except for the Archive section. In the following paragraphs we describe the different sections in more detail.

5.2 The Archive Section

The Archive section must be the first sub-element of the *febio_restart* root element. This section defines the name of the binary dump file:

```
<Archive>archive.dmp</Archive>
```

This file will be created by FEBio when requested by the user and contains the solution of the analysis up to the last converged time step.

5.3 The Control Section

The following control parameters can be redefined:

Parameter	Description
dtol	convergence tolerance for displacements
etol	convergence tolerance for energy
rtol	convergence tolerance for residual
lstol	line search tolerance
max_refs	maximum number of stiffness reformations
max_ups	maximum number of BFGS updates
restart	restart file generation flag
plot_level	defines the frequency of the plot file generation

5.4 The LoadData Section

In the LoadData section some or all of the load curves can be redefined, or new load curves can be added. The syntax is identical to the LoadData section of the FEBio input file:

```
<LoadData>
  <loadcurve id="1">
    <loadpoint>0, 0</loadpoint>
    ...
    <loadpoint>1, 0.54</loadpoint>
  </loadcurve>
</LoadData>
```

In this case, the loadcurve *id* is the loadcurve number of the loadcurve that the user wishes to redefine.

New loadcurves can be added as well. This is useful when in addition adding new Step sections, where new boundary conditions are defined. When adding new loadcurves, make sure to continue the numbering of the parent input file. That is, if the last loadcurve of the parent input file has and id of n, then the first new load curve defined here must have id of n+1.

5.5 The Step Section

The Step section can be used to add additional analysis steps to the model. These steps are executed after the initial model has completed. This section cannot be used to modify the steps defined in the parent file. See chapter 5.6.2 for more information on the Step section or multi-step analyses in general.

Using the Step section, additional boundary conditions, loads, contact definitions, etc. can be added, just like in a regular model input file. The syntax is the same as the Step section in the regular model input file. The only difference is that the type attribute is required to define the type of analysis. The type has the same role as the Module section in the regular FEBio input file.

5.6 Example

5.6.1 Example 1

The following example defines a restart input file. No parameters are redefined. Only the mandatory *Archive* element is defined. In this case the analysis will simply continue where it left off:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<febio_restart version="1.0">
  <Archive>out.dmp</Archive>
</febio_restart>
```

5.6.2 Example 2

In the following example an additional step is defined, which defines a new boundary condition and a new loadcurve.

```
<?xml version="1.0" encoding="utf-8"?>
<febio_restart version="2.0">
  <Archive>out.dmp</Archive>
  <Step type="solid">
    <Control>
      <time_steps>10</time_steps>
      <step_size>0.1</step_size>
    </Control>
    <Boundary>
      <prescribe bc="x" node_set="set1">
         <scale lc="2">1.0</scale>
      </prescribe>
    </Boundary>
  </Step>
  <LoadData>
    <loadcurve id="2" type="linear">
      <point>1, 0</point>
      <point>2, 1</point>
    </loadcuve>
  </LoadData>
</febio_restart>
```

Notice the “type” attribute in the Step section. This serves a similar purpose as the Module section in the FEBio input file and defines the solver that FEBio will use to solve this step. This attribute is required when defining steps in the restart file. (The Module section is not supported in the restart input file.)

The prescribed boundary condition references a node set named “set1”. This node set must be defined in the parent input file. No new node sets (or surfaces, etc.) can be defined in the restart input file.

```
Multi-Step Analysis
```

A multi-step analysis is defined using multiple steps, where in each step the user can redefine control parameters and boundary conditions. This is useful, for instance, for defining time-dependant boundary conditions or for switching between different analysis types during the simulation.

Multi-step models require a slightly different file organization compared to single-step models. More specifically, the Control section is not specified at the top of the input file. Instead, a *Step* section is added at the bottom of the file for each step and a *Control* section is defined for each step.

5.7 The Step Section

The multi-step analysis feature introduces a new section to the input file. Each step requires its own *step* section, preferably at the bottom of the input file. In this step section, the user can redefine the control section and the boundary section. The following format is suggested when defining a multi-step analysis:

```
<febio_spec version="2.5">
  <Module type="solid"/>
  <Material>
    <!-- materials go here -->
  </Material>
  <Mesh>
    <!-- mesh goes here -->
  </Mesh>
  <MeshDomains>
    <!-- mesh domains go here -->
  </MeshDomains>
  <Boundary>
    <!-- global boundary conditions -->
  </Boundary>
  <LoadData>
    <!-- load curve data goes here -->
  </LoadData>
  <Step>
    <Control>
      <!-- local control settings -->
    </Control>
    <Boundary>
      <!-- local boundary conditions -->
    </Boundary>
  </Step>
</febio_spec>
```

The first part of the file looks similar to a normal input file, except that the control section only is not specified. Also, the Boundary, Loads, Constraints, Contact, sections should only contain global boundary conditions.

At the end of the file the user defines as many Step sections as needed. In each Step section, the user can now define the control parameters and boundary conditions.

5.7.1 Boundary Conditions

In a multi-step analysis boundary conditions can be applied that are only active during the step. This applies to the *Boundary*, *Loads*, *Contact* and *Constraints* section of the FEBio input file. These sections can thus be placed inside the *Step* section to define a boundary condition that is only active during the step. If one of these sections is defined before the first *Step* section, the corresponding boundary conditions remain enforced during all the steps.

5.7.2 Relative Boundary Conditions

Some boundary conditions can be defined as relative boundary conditions. This means that the corresponding conditions will be applied to the final configuration of the previous step and not to the original reference configuration. For example, if a prescribed displacement is defined as relative the displacement will be taken with respect of the positions of the final configuration. This makes it possible to switch between load and displacement controlled boundary conditions in multi-step analyses.

5.8 An Example

The following example illustrates the use of the multi-step feature of FEBio. This problem defines two steps. In the first step, a single element is stretched using a prescribed boundary condition. In the second step, the boundary condition is removed and the analysis type is switched from quasi-static to a dynamic analysis. Note the presence of the global fixed boundary constraints, which will remain enforced during both steps:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<febio_spec version="3.0">
  <Module type="solid"/>
  <Material>
    <material id="1" name="material1" type="neo-Hookean">
      <density>1.0</density>
      <E>1</E>
      <v>0.45</v>
    </material>
  </Material>
  <Mesh>
    <Nodes>
      <node id="1">-2.0,-0.5, 0.0</node>
      <node id="2">-2.0,-0.5, 1.0</node>
      <node id="3">-2.0, 0.5, 0.0</node>
      <node id="4">-2.0, 0.5, 1.0</node>
      <node id="5"> 2.0,-0.5, 0.0</node>
      <node id="6"> 2.0,-0.5, 1.0</node>
      <node id="7"> 2.0, 0.5, 0.0</node>
      <node id="8"> 2.0, 0.5, 1.0</node>
    </Nodes>
    <Elements name="Part1" type="hex8">
```

```
      <elem id="1">1,5,7,3,2,6,8,4</elem>
    </Elements>
    <NodeSet name="set1">
      <node id="1"/>
      <node id="2"/>
      <node id="3"/>
      <node id="4"/>
    </NodeSet>
    <NodeSet name="set2">
      <node id="1"/>
      <node id="2"/>
      <node id="5"/>
      <node id="6"/>
    </NodeSet>
    <NodeSet name="set3">
      <node id="1"/>
      <node id="3"/>
      <node id="5"/>
      <node id="7"/>
    </NodeSet>
    <NodeSet name="set4">
      <node id="5"/>
      <node id="6"/>
      <node id="7"/>
      <node id="8"/>
    </NodeSet>
  </Mesh>
  <MeshDomains>
    <SolidDomain name="Part1" mat="material1"/>
  </MeshDomains>
  <Boundary>
    <bc type="fix" node_set="set1">
      <dofs>x</dofs>
    </bc>
    <bc type="fix" node_set="set2">
      <dofs>y</dofs>
    </bc>
    <bc type="fix" node_set="set3">
      <dofs>z</dofs>
    </bc>
  </Boundary>
  <LoadData>
    <load_controller id="1" type="loadcurve">
      <points>
       <point>0,0</point>
       <point>1,0.1</point>
      </points>
    </load_controller>
```

```
  </LoadData>
  <Step id="1">
    <Control>
      <time_steps>10</time_steps>
      <step_size>0.1</step_size>
    </Control>
    <Boundary>
      <bc type="prescribe" node_set="set4">
        <dof>x</dof>
     <scale lc="1">1.0</scale>
      </bc>
    </Boundary>
  </Step>
  <Step id="2">
    <Control>
      <time_steps>50</time_steps>
      <step_size>0.5</step_size>
      <analysis>dynamic</analysis>
    </Control>
  </Step>
</febio_spec>
```

Chapter 6

Parameter Optimization

This chapter describes FEBio's parameter optimization module. This module tries to estimate model parameters by solving an inverse finite element problem, where the "solution" of the problem is known, and the problem's model parameters are sought. In this case, the solution will often be an experimentally determined reaction force curve, and the unknown parameters are the material parameters that will recreate the reaction force curve by solving a forward FE problem. Another common application is determining the model parameters that achieve a desired load, displacement, or other goal.

In any case, the opimization module tries to minimize an objective function of the form,

$$\varphi(\mathbf{a}) = \sum_{i=1}^{n} [y_i - f(x_i; \mathbf{a})]^2 .$$

Here, the (x_i, y_i) are user-defined data pairs and $f(x; \mathbf{a})$is the function that extracts the corresponding data from the model. The optimization module tries to find the model parameters **a** that minimize the function φ. It does this by repeatedly evaluating the function f, which will usually call FEBio to solve a forward FE problem.

The optimization module requires a separate input file that describes all the information needed for solving an optimization problem. This input file is described next.

6.1 Optimization Input File

Like all FEBio input files, the parameter optimization input file is an xml-formatted text file. The following sections are defined:

Task optional section defining the task that is executed to solve the FE problem.

Options optional section defining the optimization control parameters.

Objective defines the objective function that will be minimized.

Parameters defines the model parameters that are to be determined.

Constraints defines linear constraints for the model parameters (requires a solution method that supports linear constraints).

In the following paragraphs each section will be explained in detail.

6.1.1 Task Section

The optional Task section can be used to define the task that is executed by FEBio when solving the FE model. By default, FEBio will solve the standard forward solver, but if needed, a custom task can be selected.

6.1.2 Options Section

This section defines the control parameters for the optimization. The options that can be defined will depend on the chosen optimization method, which is set with an attribute of the Options section. Currently the two implemented optimization methods are the "Levenberg-Marquardt" method (type="levmar") and the "Constrained Levenberg-Marquardt" method (type="constrained levmar"). Documentation for the Constrained Levenberg-Marquardt method can be found at http://users.ics.forth.gr/~lourakis/levmar/.

Note that this section is optional. When omitted, default values for the control parameters are chosen. The following parameters can be defined.

Parameter	Description	Default
obj_tol	Convergence tolerance for objective function. (1)	0.001
f_diff_scale	Forward difference scale factor (2)	0.001
log_level	Sets the amount of output that is generated on screen and in the logfile by the FEBio solver (3)	LOG_NEVER
tau	Step size scale factor (4)	1.0e-3
print_level	Sets the amount of output generated by the optimization module (5)	PRINT_ITERATIONS

For example,

```
<Options type="constrained levmar">
  <obj_tol>0.001</obj_tol>
  <f_diff_scale>0.001</f_diff_scale>
  <print_level>PRINT_ITERATIONS</print_level>
</Options>
```

Comments:

1. The objective function that is to be minimized is a function of the form:

$$\varphi(\mathbf{a}) = \sum_{i=1}^{n} [y_i - f(x_i; \mathbf{a})]^2 .$$

   Here, $f(x; \mathbf{a})$ is the function that describes the model, $\mathbf{a}$ is a vector with the (unknown) model parameters and the (x_i, y_i) are the user-defined data that approximates the ideal model.

2. The optimization method currently implemented requires the calculation of the gradient of the model function f with respect to the model parameters $\mathbf{a}$. Since this gradient is not known,

it will be approximated using forward differences. For example, the k-th component of the gradient is approximated as follows.

$$\frac{\partial f}{\partial a_k} \approx \frac{1}{\delta a_k} \left[f\left(a_1, \cdots, a_k + \delta a_k, \cdots, a_m\right) - f\left(a_1, \cdots, a_k, \cdots, a_m\right) \right]$$

The value for $\delta a_k$is determined from the following formula.

$$\delta a_k = \varepsilon \left(1 + a_k\right)$$

where, $\varepsilon$is the forward difference scale factor which can be set by the user with the *fdiff_scale* option.

3. The *log_level* allows the user to control exactly how much output from the time iterations of each optimization iteration is written to the screen and logfile. The following values are allowed:

Value	Description
LOG_DEFAULT	Use default settings (may be omitted)
LOG_NEVER	Don't generate any output
LOG_FILE_ONLY	Save to the logfile only
LOG_SCREEN_ONLY	Only print to the screen
LOG_FILE_AND_SCREEN	Save to the logfile and print to the screen

4. The step size scale factor *tau* can be set as an input only for the Constrained Levenberg-Marquardt method. It scales the initial guess for the damping parameter.

5. The *print_level* sets how much output is generated during the optimizations. In particular, it controls if the objective function values are printed are not. The following values are allowed:

Value	Description
PRINT_ITERATIONS	Print minimal iterations info
PRINT_VERBOSE	Print a lot of information, incl. objective function values

6.1.3 Parameters Section

This section defines the material parameters that are to be determined. Each parameter is defined using the *param* element:

```
<Parameters>
  <param name="[name]">[guess], [min], [max], [scale]</param>
</Parameters>
```

The *name* attribute gives the name of the parameter that is to be determined. The following section describes the format to reference a model parameter. Each parameter takes four values: [guess] is the initial guess for this parameter, [min] and [max] are the minimum and maximum values respectively for this parameter, and [scale] is a representative scale (magnitude) for this parameter (although the precise interpretation of this parameter depends on the particular solver). This value

is used to normalize the optimization parameter and improve convergence. If not specified by the user, it defaults to the initial guess.

For example, to optimize the material parameters of a neo-Hookean solid, named *mat1,* use the following syntax.

```
<Parameters>
  <param name="fem.material('mat1').E">1.0, 0.0, 5.0, 1.0</param>
  <param name="fem.material('mat1').v">0.1, 0.0, 0.5, 1.0</param>
</Parameters>
```

This example defines two material parameters. The first component of the name (here *mat1*) is the name of the material as defined in the model input file. The second component (here *E* and *v*) are the names of the material parameters. See Appendix A for more information how to reference model parameters.

6.1.4 Objective Section

This section defines the functional model that is used to evaluate the objective function (i.e. the function f above). There are currently two functional models supported, namely the "data-fit" and "target". They will be described separetely below.

6.1.4.1 The data-fit model

The data-fit model tries to fit predicted FE data to a user-defined data curve of time-value pairs. The data curve usually represents some experimentally obtained result, e.g. reaction force, as a function of time. The data-fit model needs a data source, i.e. a function for extracting the model data, and the data curve.

```
<Objective type="data-fit">
  <fnc type="[enter type]">
    ...
  </fnc>
  <data>
    <pt>0, 0</pt>
    ...
    <pt>1, 1</pt>
  </data>
</Objective>
```

The data source is defined by the type attribute of the fnc tag. There are currently two supported values.

- *parameter*: The function will track the time evolution of a model parameter.
- *filter_positive_only*: Another data source is needed to extract model data (e.g. parameter), but only positive values are returned. If the model parameter's value was negative, zero will be returned by the function.

In the case of *parameter*, a child element defines the parameter that will act as the data source for the objective function.

```
<fnc type="parameter">
  <param name="fem.rigidbody('rigid').Fz"/>
</fnc>
```

This defines the data function as a function of time. You can also change the ordinate of the function to create other functional dependencies. For example, the following creates a load-displacement curve for a rigid body.

```
<fnc type="parameter">
  <ordinate name="fem.rigidbody('rigid').position.x"/>
  <param name="fem.rigidbody('rigid').Fz"/>
</fnc>
```

6.1.5 Constraints Section

The Constrained Levenberg-Marquardt method allows linear constraints on the material parameters. If $\mathbf{a}$ is the material parameter vector, then the linear constraint is of the form:

$$c_1 a_1 + c_2 a_2 + ... + c_n a_n + b = 0 \quad .$$

The coefficients $c_1, c_2, ..., c_n, b$ are the inputs of the constraint tag. For example, if the linear constraint is $2a_1 - a_2 + 3 = 0$, then the Constraints section would be:

```
<Constraints>
  <constraint>2, -1, 3</constraint>
</Constraints>
```

6.2 Running a Parameter Optimization

As explained above, a parameter optimization problem is described using two input files. First, a standard FEBio input file that defines the mesh, materials, boundary conditions, etc. The second input file describes the parameter optimization data, such as the objective and which model parameters are to be optimized. The format of the second file is described above. A parameter optimization can only be initiated from the command line. For example:

```
>febio -i model.feb -s optim.feb
```

The output of a parameter optimization analysis is a log file that contains the screen output of the FEBio run as well as the optimized parameter values.

6.3 An Example Input File

Below follows a complete example of an optimization input file.

```
<?xml version="1.0"?>
<febio_optimize version="2.0">
  <Options>
    <obj_tol>0.001</obj_tol>
    <f_diff_scale>0.001</f_diff_scale>
  </Options>
  <Parameters>
    <param name="fem.material[0].E">1, 0, 5</param>
    <param name="fem.material[0].v">-0.5, 0, 0.5</param>
  </Parameters>
  <Objective type="data-fit">
    <fnc type="parameter">
      <param name="fem.rigidbody('rigid').Fz"/>
    </fnc>
    <data>
      <point>0.0, 0</point>
      <point>0.5, 1</point>
      <point>1.0, 2</point>
    </data>
  </Objective>
</febio_optimize>
```

Comments:

1. Notice that the xml root element is *febio_optimize* for the optimization input file. The version number has to be 2.0 (the 1.0 version is no longer supported).
2. The FEBio input file that contains the actual FE model data has to defined on the command line using the -i command option. This file is a standard FEBio input file that defines all geometry, materials, boundary conditions and more.
3. The initial values of the parameters are defined in the optimization input file. The values in the model input file are ignored.
4. The *Options* section is included here, but can be omitted. If omitted default values will be used for all control parameters.

Chapter 7

Troubleshooting

Running a nonlinear finite element analysis can be a very challenging task. The large deformations and complex constitutive models can make it very difficult to obtain a converged solution. There are many causes for nonconvergence, ranging from element inversions, material instability, failure to enforce contact constraints and many more. Sometimes it is possible that FEBio gives you a converged solution, but the solution is meaningless or at least not what was expected.

Fortunately, many of these issues can be prevented or solved with little effort. This chapter discusses some strategies to prevent common problems and to troubleshoot a problematic run. It offers some sanity checks before you run your model which can save you a lot of frustration down the road. And when things do go bad, we hope that the strategies suggested here may prove helpful.

However, keep in mind, that the finite element method cannot solve all problems. It is a very powerful numerical method, but with limitations. Understanding these limitations and how they affect your modeling work is crucial in becoming a good analysist.

7.1 Before You Run Your Model

In this section we'll discuss what a well-defined finite element model is and some things you may need to check before you run your model in FEBio.

A well-defined finite element model contains a finite element mesh, a valid material and properly defined boundary and contact conditions in order to define a unique solution to the problem under study. We will look at each of these requirements in more detail in the following sections.

7.1.1 The Finite Element Mesh

A finite element mesh is required to solve a problem with FEBio. The mesh defines a discretization of the problem domain in nodes and connected elements. FEBio only supports certain elements and thus the mesh must be composed of elements from this set. See Section 3.6.2 for a discussion of the supported elements. In addition, FEBio assumes a specific ordering of the nodes of an element. FEBio cannot discover if the nodes are in the correct order, but if they are not, FEBio will most likely have trouble converging or throw negative jacobians. If FEBio discovers negative jacobians before the first time step, it is likely that the nodes of the elements are not defined in the proper order.

For shell elements, the initial thickness of an element is also important. When elements are too thick (the thickness is of the same order as the element size), FEBio may complain about negative

jacobians. This may be particularly a problem in areas of high curvature. The only solution around this issue might be to remesh the problematic area.

7.1.2 Materials

A material in FEBio defines the constitutive response of the domain to which the material is assigned. See Chapter 4 for a detailed list of all the available materials in FEBio. It is important to understand that the module defines which materials you can use. For example, the biphasic material cannot be used in the *solid* module. Although some cases of invalid material use are caught, in many situations the resulting behavior is undefined. The following table shows a list of some of FEBio's special materials and the modules in which they can be used.

Material	Solid	Biphasic	Solute	Multiphasic	Heat
biphasic		**YES**	**YES**	**YES**	
biphasic-solute			**YES**	**YES**	
triphasic			**YES**	**YES**	
multiphasic				**YES**	
isotropic Fourier					**YES**

In addition to using the proper materials for a given module, it is also important to understand that most material parameters have a limited range in which they define valid constitutive behavior. For example, in a neo-Hookean material the Young's modulus must be positive and the Poisson's ratio must larger than -1 and less than 0.5. FEBio has most of these limits implemented in the code and will throw an error when a parameter value is defined that falls outside the valid range.

Since material parameters can be defined as functions of time through a loadcurve, FEBio will check all parameters at the beginning of each time step. When a parameter has become invalid the run will be aborted.

Some constitutive models are only valid for a limited amount of deformation. All materials in FEBio are designed for large deformation (in the sense that they are objective under arbitrary deformation), but that does not imply unlimited deformation. When the deformation becomes too large, the material response may become unphysical and although FEBio gives an answer, the result may be meaningless (see Section 7.8 for a discussion on interpreting the result). Some materials also become unstable at extremely large deformations. A classical example is the Mooney-Rivlin material. For a certain range of values of the material parameters, and under certain loading conditions, the stress-strain response can have a zero slope at large deformations. In that case, FEBio will most likely not be able to converge since the slope of the stress-strain response is used to progress towards the solution.

7.1.3 Boundary Conditions

Boundary conditions are necessary to uniquely define the solution of the problem under study. Improperly defined boundary conditions can lead to underconstrained or overconstrained problems.

If the problem is underconstrained the solution is not uniquely defined and FEBio will not be able to find a solution. The most common example of an undercontrained problem is one where the rigid body modes are not constrained. A rigid body mode is a mode of deformation that does alter the stress in the body. Affine translation and rotation of the entire mesh are two ways to introduce a rigid body mode. In a (quasi-)static finite element analysis all rigid body modes must

be properly constrained in order to find a unique solution. This can often very easily be achieved by constraining and edge or face of the model from moving at all.

If the problem is over-constrained, FEBio will usually find an answer but it is probably not the solution that was sought. The most common cause of an over-constrained model is one that has conflicting boundary conditions. For example, a force is applied to a node that is fixed.

7.2 Debugging a Model

When a model is not running as expected, the first thing to try is rerun the problem using FEBio's debug mode. Debug mode can be activated by adding a –g on the command line. For example,

```
>febio -i file.feb -g
```

When in debug mode, FEBio will do additional checks during the solution (e.g. check for NAN's, check for zeroes on the diagonal of the stiffness matrix, etc.) and will store all non-converged states to the plot file. Inspecting these non-converged states can often be useful to identify the cause of the problem. (E.g. when the model seems to disappear at some point might indicate a rigid body mode.)

Since storing all non-converged states may make the plot-file too large for post-processing, debug mode can also be turned on during the analysis. To do this, start the problem normally (without the debug flag –g). Then, right before the problem starts to fail, interrupt the run (using ctrl+c) and wait for the FEBio prompt to appear. Once it appears, enter *debug* [ENTER], and then *cont* [ENTER] to continue the run in debug mode.

7.3 Common Issues

In this section we take a look at some of the most common problems you may run into when solving a finite element problem with FEBio. We'll discuss possible causes of and solutions to these issues.

7.3.1 Inverted elements

When an element inverts, the element becomes so distorted that in certain areas of the element the Jacobian becomes zero or negative. In order to obtain a physically realistic solution, the Jacobian of the deformation must be positive at all points of the domain. Thus, when a negative Jacobian is found in an element, FEBio cannot continue. Fortunatly, FEBio's automatic time-stepping algorithm can usually circumvent this problem by cutting the time step back and retrying the step using a smaller time step. In addition, FEBio will recalculate the global stiffness matrix. The combination of a reduced time step and a refactored stiffness matrix will often be sufficient to overcome the negative Jacobian. However, when it is not, you may have run into a more serious problem. These are some of the common causes that may require additional user intervention.

7.3.1.1 Material instability

At large deformations, some materials can become unstable. This is usually caused by a softening of the material at large deformations. When the material softens too much the global stiffness

matrix can become ill-conditioned and FEBio will not be able to find the correct solution. Unfortunately, there is no easy solution around this issue and you may need to consider using a different constitutive model.

7.3.1.2 Time step too large

Altough the auto-time stepper will automatically adjust the time step in case of trouble, it is designed to work within user defined limits and sometimes they are not set properly to solve the problem. The most common issue is that the minimum time step is set too large. Cutting back the minimum in addition to the initial time step can often help in preventing negative Jacobians.

7.3.1.3 Elements too distorted

When elemens get too distorted they might not be able to deform any further without inverting the element. In this case, it may be necessary to adjust the mesh in the area where the elements are inverting.

7.3.1.4 Shells are too thick

A shell is an element where it is assumed that one dimension is much smaller compared to the other two directions. When the mesh is really fine, this assumption may no longer be valid and it could happen that the shell becomes too thick. When a shell gets too thick it can create negative Jacobians in the out-of-plane integration points, especially in areas of high curvature. To overcome this, you may need to remesh the affected area, adjust the shell thickness or even replace the shells with solid elements.

7.3.1.5 Rigid body modes

A rigid body mode is a mode of deformation that does not alter the stress in the body. Uniform translation or rotation of the entire model are two possible rigid body modes. In the presence of a rigid body mode, the solution is not uniquely defined and FEBio will most likely throw negative Jacobians. The solution is to identify the rigid body mode and to eliminate it by applying additional constraints to the model.

7.3.2 Failure to converge

FEBio uses an iterative method to solve the nonlinear finite element equations. This means that for each time step the solution for that step is obtained by a succession of iterations, where each iteration brings the model (hopefully) closer to the solution for that step. An iterative method requires a convergence criterium to decide when to stop iterating and FEBio uses no less than three criteria. (In biphasic and multiphasic problems additional convergence criteria are used for the pressure and concentration degrees of freedom.) The convergence norm for each of these criteria is defined by the user in the control section of the input file.

Sometimes it happens that FEBio cannot converge on a time step. We'll take a look at some of the most common causes in the next following sections. Also take a look at possible causes of element inversions above. Sometimes, the issues that cause an element inversion may also manifest themselves in convergence problems before the element actually inverts.

7.3.2.1 No loads applied

Ironically, when no loads are applied, FEBio will often struggle to find a solution. The reason (and solution!) is simple. Although no loads are applied, FEBio still performs many calculations and due to round-off errors, the result of these calculations may render the convergence norms not exactly zero. FEBio then tries to apply the convergence criteria to these really small norms and again due to round-off error will not be able to satisfy the convergence criteria.

FEBio can actually detect this situation. It looks at the residual norm and when this is smaller than a user-defined limit it assumes that no loads are present and moves on to the next time step. However, this limit is actually problem dependent and it can happen that for your particular problem the limit is set too small. In that case, the solution is to increase the limit. This can be done by setting the *min_residual* parameter in the *Control* section of the input file. For example,

```
<min_residual>1e-15</min_residual>
```

If the residual norm now drops below this value, FEBio will consider the time step converged and move on to the next time step.

7.3.2.2 Convergence Tolerance Too Tight

In some cases, the default convergence tolerances are too tight and FEBio will not be able to converge. In that case, adjusting the affected convergence norms is a possible solution. This is done by editing the corresponding norms in the Control section of the input file. However, this should only be done when no other cause can be identified for the convergence problems.

7.3.2.3 Forcing convergence

It is possible to force a time step to converge. This can be done by interrupting the run (using ctrl+c) and then enter the *conv* command at the FEBio prompt. This will force the time step to converge and FEBio will continue with the next time step. This is not a recommended practice as the solution may become unstable and in fact it is unlikely that FEBio will be able to converge any of the following time steps. However, it can be useful in some scenarios. For example, if there is no load applied in the initial time step and FEBio has trouble getting past this initial step (see Section 7.3.2.1) or when you want to store the current state to the plot file without having to rerun the problem in debug mode (although the *plot* command or *debug* command might be better alternatives).

7.3.2.4 Problems due to Contact

When contact interfaces are defined, convergence problems can often be traced back to problems with the contact interfaces. See Section 7.4 for more details on how to properly use contact interfaces in FEBio.

7.4 Guidelines for Contact Problems

FEBio offers many contact interfaces which allow the user to model complex boundary interactions. However, this capability comes at a price and the use of contact interfaces may create several

problems in the solution process. It is hoped that the guidelines presented in this section may prevent many of the most common problems with contact.

Most of the contact algorithms implemented in FEBio offer two contact enforcement methods: a penalty method and an augmented Lagrangian method. Since the strategies for these two methods are slightly different, we will look at them separately. These algorithms are discussed in much more detail in the *FEBio Theory Manual*.

7.4.1 The penalty method

The penalty method enforces contact by "penalizing" (in an energy sense) any deviation from the contact constraint. In other words, when the two contacting surfaces penetrate, a force is generated proportional to the distance of penetration, which has the effect that the surfaces will now repell each other. The strength of this repelling force is controlled by the user through the *penalty factor*.

The obvious downside of this method is that some penetration is necessary to generate the contact force. The larger the penalty factor, the smaller this penetration needs to be and thus the better the contact constraint is enforced. However, choosing the penalty factor too large may cause the problem to become unstable since the contact force (and corresponding stiffness) will dominate the other forces in the model. Choosing a good penalty factor can thus be often difficult and may require several attempts before getting it "right". To help with choosing a penalty factor, FEBio offers the *auto_penalty* option for many of its contact interfaces which will estimate a good penalty factor based on element size and initial material stiffness. However, even then it may still take a few tries before getting the penalty factor good enough.

7.4.2 Augmented Lagrangian Method

In theory, in the presence of constraints, the corresponding Lagrange multipliers must be calculated which, in the case of contact, correspond to the contact forces that enforce the contact constraint exactly. Unfortunately, the exact evaluation of these Lagrange multiplies is numerically very challenging and therefore in FEBio it was decided to evaluate these Lagrange multipliers in an iterative method, named the *Augmented Lagrangian* method. Using this method, FEBio will solve a time step several times (these iterations are termed *augmentations*), where each time the approximate Lagrange mutlipliers are updated (or *augmented*).

The obvious drawback of this method is that now each time step has to be solved several times. However, the advantage of avoiding the numerical problems of obtaining the exact Lagrange multipliers and the fact that in most contact problems very little extra work is needed to solve these augmentations, makes this method very attractive. In addition, it often gives better enforcement of the contact constraint compared to the penalty method.

So why not just use the augmented Lagrangian method? Well, often the penalty method will give good results and since the penalty method is much faster, it is often the preferred choice of many analysists.

In many cases, users are only interested in the final time step. For these users it may be of interest that it is possible to use the augmented Lagrange method only in the final time step. This can be done by defining a loadcurve for the *laugon* contact parameter. Then, define the corresponding loadcurve as zero everywhere except for the final time step. FEBio will now only use the augmented Lagrangian method in the final time step (and the penalty method all other steps).

7.4.3 Initial Separation

FEBio often struggles with problems that have an initial separation. This is especially so when the problem is force-driven, meaning that the deformation of the model is driven by a force (opposed to displacement-driven problems). In general, when the contact interface is necessary to define a well-constrained problem it is best to avoid initial separation if possible. Another way around this issue is to first use a displacement to bring the surfaces in contact and then replace the displacement with a force.

7.5 Cautionary Note for Steady-State Biphasic and Multiphasic Analyses

Biphasic, biphasic-solute and multiphasic analyses are generally transient analyses, involving mass transport (solvent and solutes) through a porous permeable domain. The default setting for these analyses is the transient mode (see Section 3.2). When a steady-state analysis is requested (*<analysis type="steady-state"/>*), the code simplifies the governing equations by setting time derivatives of the solid displacement and solute concentrations to zero. It is important to understand that this simplification is only applicable to analyses where interface conditions between sub-domains, and boundary conditions with the external environment, allow mass exchanges for the solvent and all solutes. If a domain or sub-domain is completely sealed such that it prevents solvent or solute exchanges, a steady-state analysis should not be used, as it would not capture these sealed conditions and would lead to erroneous results. For those types of problems, always use a transient analysis to obtain the correct solution. In those cases, a steady-state response may be obtained efficiently by temporarily increasing the transport properties (hydraulic permeability and solute diffusivities) by orders of magnitude via load curves, and/or by increasing the size of time steps.

7.6 Guidelines for Multiphasic Analyses

7.6.1 Initial State of Swelling

Under traction-free conditions, a multiphasic material is usually in a state of swelling due to the osmotic pressure difference between the interstitial fluid and the external environment. This osmotic pressure arises from the difference in interstitial versus external concentrations of cations and anions, caused by the charged solid matrix and the requirement to satisfy electroneutrality. An osmotic pressure difference arising from such electrostatic interactions is known as the *Donnan osmotic pressure*. When the Donnan pressure is non-zero, traction-free conditions do not produce stress-free conditions for the solid matrix, since the matrix must expand until its stressed state resists the swelling pressure.

The Donnan pressure reduces to zero when the fixed charged density is zero, or when the external environment is infinitely hypertonic (having ion concentrations infinitely greater than the interstitial fixed charge density). Since these two conditions represent special cases, it is generally necessary to devise methods for achieving the desired initial state of swelling, in an analysis where loads or displacements need to be prescribed over and above this swollen state. Swelling occurs as a result of the influx of solvent into the porous solid matrix. This influx is a time-dependent process that could require extensive analysis time. Therefore, it is computationally efficacious

to achieve the initial state of swelling by using a multi-step analysis (Chapter 5.6.2) where the first step is a steady-state analysis (Section 3.3.1). In this steady-state step, the fixed charge density may be ramped up from zero to the desired value using a load curve for that property or, alternatively, the external environmental conditions may be reduced from a very high hypertonic state down to the desired level. In the second step, prescribed displacement boundary conditions (when needed) may be specified to be of type *relative* (Section 3.10.1), so that they become superposed over and above the initial swelling state.

Example:

```
<Module type="multiphasic"/>
<!-- rest of file -->
<Step>
  <Control>
    <analysis type="steady-state"/>
    ...
  </Control>
</Step>
<Step>
  <Control>
    ...
  </Control>
  <Boundary>
    <prescribe type="relative">
      <node id="22" bc="z" lc="4">1</node>
      ...
    </prescribe>
  </Boundary>
</Step>
```

7.6.2 Prescribed Boundary Conditions

In most analyses, it may be assumed that the ambient fluid pressure and electric potential in the external environment are zero, thus $p_* = 0$ and $\psi_* = 0$, where the subscripted asterisk is used to denote environmental conditions. Since the external environment does not include a solid matrix, the fixed charge density there is zero. For example, for a triphasic analysis, $c_*^+ = c_*^- \equiv c_*$. It follows that the effective fluid pressure in the external environment is $\tilde{p}_* = -R\theta\Phi_* \sum_\alpha c_*^\alpha$ and the effective concentrations are $\tilde{c}_*^\alpha = c_*^\alpha/\hat{\kappa}_*^\alpha \tilde{c}_*^\alpha$. Therefore, in multiphasic analyses, whenever the external environment contains solutes with concentrations c_*^α, the user must remember to prescribe non-zero boundary conditions for the effective solute concentrations *and* the effective fluid pressure.

Letting $p_* = 0$ also implies that prescribed mixture normal tractions (Section 3.12.2.3) represent only the traction above ambient conditions. Note that users are not obligated to assume that $p_* = 0$. However, if a non-zero value is assumed for the ambient pressure, then users must remember to incorporate this non-zero value whenever prescribing mixture normal tractions. Similarly, users are not required to assume that $\psi_* = 0$; when a non-zero value is assumed for the electric potential of the external environment, the prescribed boundary conditions for the effective concentrations should be evaluated using the corresponding partition coefficient, $\tilde{c}_*^\alpha = c_*^\alpha/\tilde{\kappa}_*^\alpha$.

7.6.3 Prescribed Initial Conditions

When a multiphasic material is initially exposed to a given external environment with effective pressure $\tilde{p}_*$ and effective concentrations $\tilde{c}^\alpha_*$, the initial conditions inside the material should be set to $\tilde{p} = \tilde{p}_*$ and $\tilde{c}^\alpha = \tilde{c}^\alpha_*$ in order to expedite the evaluation of the initial state of swelling. The values of $\tilde{p}_*$ and $\tilde{c}^\alpha_*$ should be evaluated as described in Section 7.6.2.

7.6.4 Prescribed Effective Solute Flux

The finite element formulation for multiphasic materials in FEBio requires that the natural boundary condition for solute α be prescribed as $\tilde{j}^\alpha_n \equiv j^\alpha_n + \sum_\beta z^\beta j^\beta_n$, where $\tilde{j}^\alpha_n$ is the effective solute flux. For a mixture containing only neutral solutes ($z^\beta = 0, \forall\beta$), it follows that $\tilde{j}^\alpha_n = j^\alpha_n$.

7.6.5 Prescribed Electric Current Density

The electric current density in a mixture is a linear superposition of the ion fluxes,

$$\mathbf{I}_e = F_c \sum_\alpha z^\alpha \mathbf{j}^\alpha \,.$$

Since only the normal component $j^\alpha_n = \mathbf{j}^\alpha \cdot \mathbf{n}$ of ion fluxes may be prescribed at a boundary, it follows that only the normal component $I_n = \mathbf{I}_e \cdot \mathbf{n}$ of the current density may be prescribed. To prescribe I_n, it is necessary to know the nature of the ion species in the mixture, and how the current is being applied. For example, if the ions in the triphasic mixture consist of Na^+ and Cl^-, and if the current is being applied using silver/silver chloride (Ag/AgCl) electrodes, a chemical reaction occurs at the anode where Ag combines with Cl^- to produce AgCl, donating an electron to the electrode to transport the current. At the cathode, the reverse process takes place. Therefore, in this system, there is only flux of Cl^- and no flux of Na^+ ($j^+_n = 0$) at the electrode-mixture interface, so that the prescribed boundary condition should be $j^-_n = -I_n/F_c$. Since $z^+ = +1$ and $z^- = -1$ in a triphasic mixture, the corresponding effective fluxes are given by $\tilde{j}^+_n = 2j^+_n - j^-_n = I_n/F_c$ and $\tilde{j}^-_n = j^+_n = 0$.

7.6.6 Electrical Grounding

If a multiphasic mixture containing ions is completely surrounded by ion-impermeant boundaries it is necessary to ground the mixture to prevent unconstrained fluctuations of the electric potential. Grounding is performed by prescribing the effective concentration of one or more ions, at a location inside the mixture or on one of its boundaries corresponding to the location of the grounding electrode. The choice of ion(s) to constrain may be guided by the type of grounding electrode and the reference electrolyte bath in which it is inserted.

7.7 Guidelines for Fluid Analyses

7.7.1 Degrees of Freedom and Boundary Conditions

FEBio's fluid solver differs from most computational fluid dynamics programs by its use of fluid dilatation e^f, instead of fluid pressure p, as a nodal degree of freedom. In the *fluid* module, these two variables are related by a simple constitutive relation, $p = -K\, e^f$, where K is the fluid's bulk

modulus. The reason for selecting e^f instead of p is that the dilatation is a kinematic measure, just like the fluid velocity $\mathbf{v}^f$ (the other nodal degree of freedom), whereas the pressure is a function of state (it needs to be formulated as a function of the deformation, just like the viscous fluid stress $\boldsymbol{\tau}$). The fluid Cauchy stress is given by $\boldsymbol{\sigma}^f = -p\mathbf{I} + \boldsymbol{\tau}$. The viscous stress $\boldsymbol{\tau}$ depends on the fluid rate of deformation tensor $\mathbf{D}^f$ according to a user-selected constitutive relation, such as *Newtonian fluid*.

In a fluid analysis, the user may prescribe any of the components of $\mathbf{w}$ as an essential boundary condition, or the corresponding component of the viscous traction $\mathbf{t}^\tau = \boldsymbol{\tau} \cdot \mathbf{n}$ as a natural boundary condition ($\mathbf{n}$ being the normal to the boundary surface). When neither a component of $\mathbf{w}$ nor the corresponding component of $\mathbf{t}^\tau$ is prescribed explicitly, the latter is naturally assumed to be zero. Similarly, the user may either prescribe e^f as an essential boundary condition (which is equivalent to prescribing $p = -Ke^f$), or $w_n = \mathbf{w} \cdot \mathbf{n}$ as a natural boundary condition. When neither is prescribed explicitly, it is naturally assumed that $w_n = 0$. Natural boundary conditions are useful for creating symmetry planes in fluid analyses, where the normal fluid velocity and the viscous traction are zero: On those symmetry planes, no boundary conditions should be specified.

It is noteworthy that the fluid formulation in FEBio allows the prescription of the nodal value of $\mathbf{w}$ as an essential boundary condition, and the surface value of w_n as a natural boundary condition. On boundaries where the fluid velocity is completely prescribed, i.e., when normal and tangential components are known (and not zero), prescribing $\mathbf{w}$ and w_n instead of just $\mathbf{w}$ produces the best computational outcome. In those cases, the user should use the *fluid velocity* surface load, which combines both boundary conditions (Section 3.12.2.13). If the user only wants to prescribe a known normal velocity w_n and leave the tangential velocity unspecified, use the *fluid normal velocity* surface load (Section 3.12.2.12); this surface load also provides the option of setting the tangential fluid velocity to zero. Finally, if the user wants the velocity to remain normal to the selected surface (e.g., an inlet or outlet surface on which e^f is prescribed or fixed), but does not know the velocity magnitude *a priori*, use the *normal fluid velocity* constraint (Section 3.14.4) to enforce this condition.

A viscous fluid satisfies the no-slip condition on a physical boundary surface. This means that $\mathbf{w} = \mathbf{0}$ on no-slip boundaries. This boundary condition can be enforced simply by fixing the three components of $\mathbf{w}$ (Section 3.10.2) and not specifying any value for e^f on that surface (which naturally enforces $w_n = 0$).

Computational fluid dynamics analyses are often performed over a mesh that truncates the real fluid domain. Thus, fluid may enter the finite element domain across some upstream inlet boundary and leave the domain across some downstream outlet boundary. The exact flow conditions on these boundaries may not be known, thus they have to be approximated using best guesses. Arguably, the viscous traction $\mathbf{t}^\tau$ is the least intuitive boundary condition to guess. On an outlet boundary, it is necessary to prescribe or fix the dilatation e^f to overcome the natural boundary condition $w_n = 0$. However, in most cases the tangential components of $\mathbf{w}$ on that boundary are not known, therefore they cannot be fixed or prescribed, leading to the natural condition $\mathbf{t}^\tau = \mathbf{0}$. This natural condition may work fine in some cases, but it will often fail numerically when vortices being shed inside the finite element domain try to cross the outlet boundary. In those cases, consider using the *fluid backflow stabilization* (Section 3.12.2.10) and *fluid tangential stabilization* (Section 3.12.2.11) surface loads, which prescribe a velocity-dependent viscous traction $\mathbf{t}^\tau$.

Similarly, on an inlet boundary that shares an edge with a no-slip surface, prescribing the fluid velocity $\mathbf{w}$ on the inlet boundary may not accurately reproduce the velocity profile in the boundary layer that would be produced on the adjoining no-slip surface. This potential mismatch could result in numerical instabilities; in such cases, prescribing a dilatation e^f on the shared edge may mitigate this issue.

7.7.2 Biased Meshes for Boundary Layers

In fluid analyses, boundary layers will form in the vicinity of no-slip boundaries, where the velocity magnitude varies rapidly with the distance from a no-slip surface. The thickness of boundary layers decreases with increasing Reynolds number. To capture these boundary layers accurately in a fluid finite element analysis, it is necessary to refine the mesh to produce thinner elements closer to the no-slip boundaries. This is done most conveniently by using mesh biasing tools, available in various meshing software programs, or post-hoc boundary-layer meshing tool that modify an existing mesh. Both of these options are available in FEBioStudio. Boundary layer meshing should always be used in fluid analyses in FEBio. Whereas other finite element codes employ numerical stabilization techniques that partially alleviate the need for biased meshes, FEBio does not employ such techniques. Therefore, using uniform finite element meshes may fail to produce numerical convergence, even in some seemingly simple problems. Users should keep in mind that biased meshes don't necessarily require more nodes and elements, therefore there is no automatic computational cost for using biased meshes.

7.7.3 Computational Efficiency: Broyden's Method

Fluid analyses produce a non-symmetric stiffness matrix and the resulting system of equations may be efficiently solved using Broyden's quasi-Newton method, where an approximation to the matrix inverse is produced at each iteration after the first full-Newton iteration of a time step. In fluid analyses, it is often possible to achieve convergence at each time step without having to perform additional full-Newton updates. Therefore, it is recommended to set *max_updates* (Section 3.3) to a large number (e.g., 50), along with setting *diverge_reform* to 0 (false), which leads to a more efficient solution scheme. A further advantage arises in fluid analyses since the mesh remains invariant over time: it is often possible to continue using Broyden updates even across time steps, without performing a full-Newton iteration at the start of that step, by setting *reform_each_time_step* to 0 (false). In that case, the solver will continue using Broyden updates up to the value of *max_updates*, before performing a full Newton update.

7.7.4 Dynamic versus Steady-State Analyses

FEBio runs fluid analyses in dynamic mode by default, because many fluid flow problems do not have a steady-state solution, since the governing equations are nonlinear. For example, many flows may exhibit vortex shedding as fluid flows across an obstacle, such as a flow constriction or a solid body. Even if some form of periodicity emerges under specific flow conditions, as in the von Karman vortex street, the corresponding solution is not in steady state. However, for some low Reynolds number laminar flows, a steady-state response may exist and FEBio will attempt to find that solution when using analysis type "steady-state" (Section 3.3). The user should be aware that, under steady-state analyses, the solution may not necessarily converge as efficiently to the final solution as would a dynamic analysis that allows the solution to reach steady state after a sufficiently long time. The best choice of analysis type for steady-state problems may need to be determined by trial and error.

7.7.5 Isothermal Compressible Flow versus Acoustics

The governing equations for fluid flow in FEBio represent isothermal conditions, thus eliminating temperature as a variable in the numerical analysis. Since the fluid solver accommodates some

measure of fluid compressibility (via the fluid dilatation variable e^f), it is possible to solve for pressure wave propagation in fluids using this formulation. However, from a theoretical perspective, it should be recognized that the speed of sound (i.e., the wave speed) in isothermal (constant temperature) flow is different from the speed of sound in isentropic (constant entropy) flow. The field of acoustics typically examines pressure wave propagations under isentropic conditions, which are found to be more consistent with experimental measurements of the speed of sound in air. Therefore, the FEBio fluid solver may not produce realistic wave speeds when simulating acoustics. A fluid solver for isentropic flow may be developed for FEBio in the future.

7.7.6 Fluid-Structure Interactions

Fluid-structure interactions (FSI) may be modeled in FEBio using the *fluid-FSI* module (Section 3.2). In an FSI analysis the finite element mesh defining the fluid domain is deformable, so that the shape of the fluid domain does not have to remain fixed over time. The fluid flows through the deforming mesh, just as it does in standard computational fluid dynamics (CFD) analyses with fixed meshes. The deformation of the fluid domain may be controlled by prescribing suitable boundary conditions (so-called moving boundary problems) and by interactions with solid domains. For example, fluid may flow inside a flexible tube and the fluid pressure may cause the tube to expand or contract; the tube itself may be pinched at some location, reducing the cross-section through which fluid flows. The tube wall is a deformable solid domain which may be modeled in FEBio using any of the solid material models described in Sections 4.1 through 4.6. The inner tube (the fluid domain) should be modeled as a *fluid-FSI* material (Section 4.13.3).

In FEBio, a *fluid-FSI* material is modeled as a specialized fluid-solid mixture. It requires the user to define a *fluid* material from the same list as those available for CFD analyses (Section 4.13). It also requires the user to define a *solid* material to regularize the mesh deformation. The *solid* material of a *fluid-FSI* material is massless (the *density* value entered by the user is ignored and reset internally to zero). Among all the choices available in Section 4.1, it is recommended to use the *neo-Hookean* elastic solid (Section 4.1.3.17), setting Poisson's ratio ν to zero and Young's modulus E to a very low value (a few orders of magnitude smaller than the moduli of surrounding solid domains).

The degrees of freedom at each node of a fluid-FSI domain consist of the components of the solid displacement $\mathbf{u}$ (which describe the mesh deformation), the fluid velocity $\mathbf{w}$ relative to the solid, and the fluid dilatation e^f. Essential boundary conditions may be prescribed on any of these degrees of freedom. For example, in a moving boundary problem, the motion of a boundary may be prescribed by setting the relevant components of $\mathbf{u}$. A no-slip boundary may be defined by simply setting $\mathbf{w} = \mathbf{0}$, regardless of the motion of that boundary. In general, all boundary conditions described for CFD analyses in Section 7.7.1 may be applied identically to FSI analyses.

In FEBio 2.8 the mesh of a *fluid-FSI* domain must be continuous with the mesh of surrounding solid domains. The surface between fluid and solid domains, which consists of the shared faces of adjoining finite elements from each domain, is called the FSI interface. Because the mesh is continuous, the solid displacement and the solid component of the traction are automatically continuous across FSI interfaces. However, the fluid component of the traction in the *fluid-FSI* domain must be explicitly transferred to the solid domain across the FSI interface. This is done by prescribing a *fluid-FSI traction* on that interface (Section 3.12.2.16). This surface load does not require any user-defined parameters; its sole purpose is to identify those FSI interfaces where the fluid traction must be properly transferred to the surrounding solid domain. Omitting this boundary condition means that the fluid traction (i.e., the fluid pressure and the normal and tangential viscous components of the fluid stress) have no effect on this interface; the interface may still deform in

response to the motion of the solid domain. For example, when a fluid interacts with a rigid solid domain whose motion is entirely prescribed, it is not necessary to apply a *fluid-FSI traction* at the interface between the fluid and rigid solid domains.

A fluid-FSI traction is also required on free fluid surfaces, such as the surface of a fluid in open channel flow, in order to properly capture the motion of that surface (such as waves). This condition is required since the net traction $\mathbf{t}$ on a free surface is zero. As the fluid-FSI domain is modeled as a specialized solid-fluid mixture, the net traction consists of the sum of solid and fluid tractions, $\mathbf{t} = \mathbf{t}^s + \mathbf{t}^f$. Setting $\mathbf{t}$ to zero produces a traction $\mathbf{t}^s = -\mathbf{t}^f$ on the solid mesh, allowing it to deform to the proper shape.

Here are a few cautionary notes to keep in mind when running FSI analyses: (1) Depending on the problem being analyzed, fluid-structure interactions may cause significant mesh deformations that lead to mesh distortion. As of FEBio 2.8 adaptive meshing is not yet available, therefore analyses and meshes need to be designed to minimize this effect or to terminate before the solution becomes too corrupted. (2) It is possible to pinch a solid domain that surrounds a fluid domain until the flow cross-section has reduced considerably; however it is not possible to completely shut off the flow, as this would require reducing the volume of some finite elements to zero. (3) While it is possible to model the deformation of free fluid surfaces, such as the formation of surface waves in open channel flow or the deformation of fluid blobs floating in a gravity-free environment, it is not possible to model the separation of such fluid domains into sub-domains such as spraying fluid droplets; this means that analyses where such phenomena are expected to happen will likely fail. (4) Whereas standard CFD analyses may be jump-started by prescribing a relatively large fluid velocity at the very first time step of an analysis, these types of boundary conditions may lead to dynamic oscillations and potential instabilities in an FSI analysis; therefore, users must be more considerate when prescribing boundary conditions for FSI analyses.

7.8 Understanding the Solution

Okay, FEBio found a solution. Great, but how do you know it is the right one? Well, it turns out this is in fact a harder question than it may seem. In any finite element model there are numerous assumptions and approximations and trying to discuss all of these is outside the scope of this section. Instead, we'll look at some of the most typical problems that FEBio users have run into.

7.8.1 Mesh convergence

The solution calculated by FEBio only applies to the mesh for which it was solved. However, the "exact" solution must be independent of the mesh and therefore a mesh convergence study is almost always necessary to make sure the FEBio solution is close to this exact solution. In practice this means that a model must be run several times with an increasingly finer mesh to find out at which mesh density the FEBio solution no longer changes.

7.8.2 Constraint enforcement

FEBio uses many iterative algorithms for enforcing constraints. For each of these contraints the user must verify that the solution indeed satisfies these constraints sufficiently. The two most common constraints used in FEBio are incompressibility and contact.

For uncoupled materials, incompressibility (for hexahedral elements) is handled in FEBio using a three-field formulation in addition to the enforcement of the incompressibility constraint. This

constraint is usually enforced using a penalty formulation (although an augmented Lagrangian method is also available). To inspect whether the incompressibility constraint is satisfied sufficiently the user can look at the volume ratio which has to be close to one. If it deviates from one too much the user needs to increase the "bulk modulus" of the material.

For coupled materials, incompressibility is not treated explicitly and care must be taken when using coupled materials in a near-incompressible regime (e.g. setting the Poisson's ratio too close to 0.5 for a neo-Hookean material). In that case, the solution will most likely "lock" which manifests itself in displacements that are too small. Inspection of the volume ratio may not be sufficient to identify locking. However, a mesh convergence study will often help in identifying this problem.

When a contact constraint is not sufficiently enforced, the contacting surfaces will have penetrated. This problem is usually identified easily by looking at the deformed model in a post-processing software (e.g. PostView). Increasing the penalty factor and/or decreasing the augmented Lagrangian tolerance should solve this problem.

7.9 Guidelines for Using Prestrain

There are a variety of ways in which prestrain can be added to an FEBio model, but the recommended approach – a two-step approach – is outlined here.

In the first step, the prestrain is enforced on the model. This is accomplished by making sure the part that will be prestrained uses the prestrain elastic material (or uncoupled prestrain elastic for uncoupled hyperelastic materials). A suitable prestrain generator must be defined as well. In addition, one of the update rules can be specified as a nonlinear constraint in order to modify the effective prestrain field. The boundary conditions in this step should be minimal but sufficient to ensure a well-defined finite element problem.

After the first step converges, the model is successfully prestrained. However, depending on the application, the reference geometry could have changed and this may complicate the application of further loads (most of FEBio will still use the original geometry as the reference geometry). To eliminate this potential source of confusion, it is recommended to apply the prestrain initial condition (see chapter 4) which essentially fixes the prestrain gradient and resets the reference geometry to the current geometry. FEBio will then apply any subsequent loads to this new reference geometry. One caveat of this approach is that the plotfile still stores the original reference geometry. To prevent inconsistencies in the plotfile it is recommend suppressing the creation of the plot file in the first step. This is done by setting the following control flag in the Control section of the first step.

```
<plot_level>PLOT_NEVER</plot_level>
```

Then, in the Control section of the second step, restore the plot level value.

```
<plot_level>PLOT_DEFAULT</plot_level>
```

Now, the new reference configuration resulting after the prestrain analysis step, will be the reference configuration that is used in the plot file.

7.10 Limitations of FEBio

If you run into a problem that you can't seem to solve, maybe you ran into a limitation of FEBio. This section discusses some important limitations of the software and how they may affect the

outcome of your analysis.

7.10.1 Geometrical instabilities

A geometrical instability is a point in the solution at which several paths for continuing the solution are possible. Typical examples are buckling of a column. FEBio's Newton based solvers cannot handle buckling since usually at these points, the material's elasticity tangent is not uniquely defined. Although in some cases FEBio will be able to pass a buckling point, in most cases, FEBio will not be able to converge to a solution.

7.10.2 Material instabilities

A material instability is a point in the stress-strain response where the slope of the stress-strain curve effectively becomes zero. Since FEBio's Newton based solvers use this slope to advance the solution, a zero slope would mean an infinite step and FEBio will not be able to continue.

The slope (or more accurately the elasticity tangent tensor) does not have to be zero to cause problems. For materials that soften at large deformations, this slope may become so small that it renders the global stiffness matrix ill-conditioned. It is unlikely that FEBio will be able to continue and even if it finds a solution, it may not be useful.

7.10.3 Remeshing

FEBio is designed to solve problems that can undergo large deformations. However, when the deformations become too large it can happen that the finite element mesh cannot be distorted any further without inverting elements. In that case, FEBio will not be able to continue the solution and will most likely terminate with a negative jacobian error message.

One possible solution to this problem is to remesh the model at the point at which the deformation become too large, but currently FEBio does not have any remeshing capabilities. The only remedy at this point is to plan ahead and design your mesh in such a way that the elements will not invert in the range of deformation that you are interested in (e.g. place a butterfly mesh in sharp corners or make the mesh finer in areas of larger deformation).

7.10.4 Force-driven Problems

When the primary method of deforming the model is a force, the problem is said to be force-driven. (Opposed to a displacement-driven model where the deformation is caused by displacement boundary conditions.) Force-driven forces are inherently unstable and FEBio has limited capabilities of handling such problems[1]. The cause of this instability can easily be explained using a simple example. Imagine a box that is constrained in all directions except one. In the unconstrained direction, apply two equal but opposite forces on opposite faces. In order to prevent the box from flying away, the box must generate stresses which balance the applied forces exactly. Unfortunately, the numerical solution will only be approximate due to numerical round-off errors inherent in the calculation. Even the slightest deviation from balancing the forces exactly will create a net-force which in turn causes the model to fly off in the unconstrained direction (in which a rigid body mode now exists).

[1] As of FEBio 2.0, some features are available that may help with this issue, but they are still experimental.

Usually, these problems are circumvented by adjusting the boundary conditions so that rigid body modes cannot exist. In the previous example this can be done by only modeling half of the box and enforcing a symmetry boundary condition. However, in some cases this is not possible. This is often the case in force-driven contact problems, where the contact interface is necessary to define a well-constrained model. When there is an initial separation (or even when the surfaces have no initial overlap) the initial contact force is zero, which is equivalent to having no contact enforcement, and thus the model is under-constrained. Therefore, for force-driven contact problems it is important to have some initial contact before starting the analysis.

7.10.5 Solutions obtained on Multi-processor Machines

Although technically not a limitation of FEBio it is important that users are aware that in some cases you may get a different convergence history or sometimes even a slightly different answer when you run the same model twice on a multi-processor machine. This is caused by the fact that on multi-processor machines the same calculations can be executed in a different order and due to the accumulation of numerical round-off errors may result in slightly different answers. The type of problems that are mostly affected by this are problems that are close too being ill-conditioned. Also, problems that have many time steps or require many iterations for each time step may be affected by this.

If you experience different answers for the same problem, try running the model on just one processor (if possible). See Section 2.6 for more information on how to run FEBio on multi-processor machines.

7.11 Where to Get More Help

When you get here, you may be ready to pull all your hair out, but fret not, all is not lost. In fact, some people may have run into a similar issue and found a solution. The first place to find these people is on the FEBio user's forum (https://forums.febio.org/). This forum contains hundreds of posts by FEBio users and is monitored by the FEBio developers who will always be more than happy to help you with your problems. In addition, this forum can be used to report bugs or to request a new feature. It is the ideal portal to find help with your problems so don't hesitate to use it!

Chapter 8

Configuration File

8.1 Overview

FEBio requires a configuration file to run. The purpose of this file is to store platform-specific settings such as the default linear solver. See Section 2.5 for more information on how to use this file. This section details the format of this file.

The configuration file uses an xml format. The root element must be *febio_config*. The required attribute *version* specifies the version number of the format. Currently this value must be set to "3.0". The following elements are defined.

Parameter	Description
default_linear_solver	Set the default linear solver for the platform (1)
import	Load a plugin file (2)
set	define an alias (3)
if_debug	Process child tags only for debug versions of FEBio (4)
if_release	Process child tags only for release versions of FEBio (4)

Comments:

1. FEBio supports several linear solvers, such as Pardiso and Skyline. Not all solvers are available for all platforms. Only the Skyline solver is available for all platforms. As of version 1.2, the Pardiso solver is available on all platforms for which FEBio is distributed. See section 8.2 on how to configure the linear solvers.

2. As of FEBio 2.0 the user can create and use plugins designed for FEBio. These plugins extend the standard capabilities without the need to recompile the FEBio code. See Chapter 9 for more information on using plugins in FEBio.

3. As of FEBio 2.5 the configuration file supports aliases which can be used to define plugin paths. The *set* tag defines an alias. The name of the alias is specified via the *name* attribute. Aliases are accessed using the $(*name*) syntax. See below for an example.

4. The *if_debug/if_release* tags allow users to customize settings based on whether a debug or release version of FEBio is processing the configuration file. (Note that the debug version refers to how FEBio was compiled. It does not refer to the -g command line option.) The versions of FEBio distributed through the website are release versions. A debug version of FEBio can only be obtained by building FEBio with the _DEBUG preprocessor command.

An example configuration file that sets the default linear solver to pardiso, defines an alias, and loads a plugin.

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<febio_config version="3.0">
  <default_linear_solver type="pardiso"/>
  <set name="PluginsDir">C:\path\to\plugins</set>
  <import>$(PluginsDir)\myplugin.dll</import>
</febio_config>
```

8.2 Configuring Linear Solvers

FEBio offers several direct and iterative linear solvers that can be used to solve the linear system of equations of the FE model. Users can configure these linear solvers in the configuration file with the `default_linear_solver` tag. The particular linear solver is selected via the `type` attribute. The following table lists the possible values, the solver type, and the supported matrix format.

solver	description	type	matrix forr
pardiso	A sparse direct solver, from the MKL library. The default solver in FEBio.	direct	any
skyline	A sparse direct solver, but not as efficient as pardiso.	direct	symmetri
fgmres	An implementation of the GMRES algorithm, from the MKL library.	iterative	unsymmet
cg	An implementation of the CG algorithm, from the MKL library.	iterative	symmetri
boomeramg	An algebraic multigrid solver, from the HYPRE library.	iterative	any
schur	A block based iterative solver.	iterative	block

Iterative solvers can be configured with preconditioners, which attempt to reduce the condition number of the matrix. Preconditioning is highly recommended and often necessary for reducing the number of iterations needed by the iterative solver to converge the solution. Any of the linear solvers listed above can be used as a preconditioner. In addition, the following specialized preconditioners are also available.

preconditioner	description	matrix format
ilu0	Incomplete LU decomposition with no fill-in	unsymmetric
ilut	Incomplete LU decomposition with custom fill-in	unsymmetric
ichol	Incompletly Cholesky decomposition with no fill-in	symmetric
diagonal	Diagonal preconditioner made from the diagonal of the matrix	any

The following sections describe each of these solvers and preconditioners in more detail.

8.2.1 Pardiso

The Pardiso solver is an effecient sparse direct linear solver and is the default linear solver. FEBio uses the implementation from the MKL library. It does not require any configuration parameters. It can take symmetric, unsymmetric, and structurally symmetric sparse matrix formats.

8.2.2 Skyline

The Skyline solver was initially added for users who build their own copy of FEBio and did not have access to third party linear solvers. It is a sparse direct solver, but not as efficient as Pardiso and not recommended for large problems. When using this solver, it is highly recommended to set the `optimize_bw` flag in the model file's Control section, which attempts to minimize the matrix bandwidth. It does not require any configuration parameters and only works with symmetric matrices.

8.2.3 FGMRES

This iterative linear solver, from the MKL library, implements the GMRES algorithm, which is an efficient Krylov-based iterative solution strategy. It requires several configuration parameters, listed below, and only works with unsymmetric matrices. In the table below, **N** refers to the number of equations.

parameter	description	default
max_iter	The maximum number of iterations	min(N,150)
tol	relative residual tolerance	1e-6
abs_tol	absolute residual tolerance	1e-12
print_level	The amount of information printed (0,1, or 2)	0
fail_max_iters	Indicates whether reaching max iters is a failure or not (1)	1 (true)
pc_left	The left preconditioner	(none)
pc_right	The right preconditioner	(none)

Comments:

1. When using FGMRES as a preconditioner it is recommended to set the fail_max_iters flag to zero.

8.2.4 CG

This iterative linear solver, from the MKL library, implements the Conjugate Gradient algorithm, which is an efficient Krylov-based iterative solution strategy for symmetric systems. It requires several configuration parameters, listed below, and only works with unsymmetric matrices. In the table below, **N** refers to the number of equations.

parameter	description	default
max_iter	The maximum number of iterations	min(N,150)
tol	relative residual tolerance	1e-6
print_level	The amount of information printed (0,1, or 2)	0
pc_left	The left preconditioner	(none)

8.2.5 BoomerAMG

This solver, from the HYPRE library, is an adaptive multigrid solver. It often works better as a preconditioner to an iterative solver than as a stand-alone solver.

parameter	description	default
max_iter	The maximum number of iterations	20
tol	relative residual tolerance	1e-7
print_level	The amount of information printed (0,1, or 2)	0
max_levels	The max number of multigrid levels	25
coarsen_type	Method of grid coarsening	(library default)
use_num_funcs	Use dimensionality of solution variable in coarsening	0 (false)
relax_type	relaxation type	3
interp_type	interpolation type	6
strong_threshold	strong threshold	0.5
p_max_elmts	P max elements	4
num_sweeps	Number of sweeps	1
agg_num_levels	Aggressive number of levels	0
nodal	Nodal option	0 (false)
do_jacobi	Do jacobi preconditioning	0 (false)
fail_max_iters	Fail on max iterations (1)	1 (true)

Comments:

1. When using this solver as a preconditioner, it is recommended to set the fail_max_iters flag to 0.

8.2.6 Schur

The Schur solver is a linear solver that takes a 2x2 block structured matrix and solves the linear system by decomposing it in its Schur-complement form. Thus, instead of solving the following system directly,

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$$

it first solves for v,

$$Sv = b - CA^{-1}a$$

where $S = D - CA^{-1}B$ is the Schur complement of A. Then the Schur solver solves for u,

$$u = A^{-1}(a - Bv)$$

In order to use this solver, users need to select how they wish to solve the A-block, and how to solve the Schur complement. For the A-block users can choose any of the linear solvers listed above, either direct or iterative. For the Schur complement users can only choose a Krylov-based iterative solver (FGMRES or CG) because FEBio does not form the Schur complement explicitly.

This solver is often more effective as a preconditioner for FGMRES. In this case, the A-block and Schur complement only need to be solved approximately. See the examples section below for

some example configurations. This solver requires a block-structured matrix. In order to generate the block structure you need to set the `equation_scheme` control parameter to 1 in the model input file.

parameter	description	default
print_level	The amount of information printed (0,1, or 2)	0
schur_block	Take the Schur complement of A (=0) or D (=1)	0
do_jacobi	Do Jacobi preconditioning	0
zero_D_block	Is the D-block zero?	0 (false)
A_solver	The solver for the A-block (outside the Schur complement)	user specified
schur_solver	The iterative solver for solving Schur complement	user specified
schur_A_solver	The solver for the A block in the Schur complement	(same as A_solver)

8.2.7 Examples

Example 1. The default pardiso solver is defined in the configuration file using the following syntax. It does not require any parameters.

```
<default_linear_solver type="pardiso"/>
```

Example 2. This example shows how to set up the FGMRES solver with an ILU0 preconditioner.

```
<default_linear_solver type="fgmres">
  <max_iter>100</max_iter>
  <tol>1e-5</tol>
  <pc_left type="ilu0"/>
</default_linear_solver>
```

Example 3. This example sets up an FGMRES solver with a Schur preconditioner. For the Schur system we use pardiso for solving the A-block outside of the Schur complement and approximate the A-block inside the Schur complement with its diagonal. This solver requires a block-structured matrix. In order to generate the block structure you need to set the `equation_scheme` control parameter to 1 in the model input file.

```
<default_linear_solver type="fgmres">
 <print_level>2</print_level>
 <max_iter>100</max_iter>
 <tol>1e-5</tol>
 <abs_tol>1e-9</abs_tol>
 <pc_left type="schur">
   <print_level>0</print_level>
   <do_jacobi>0</do_jacobi>
   <A_solver type="pardiso"/>
   <schur_pc>0</schur_pc>
   <schur_A_solver type="diagonal"/>
   <schur_solver type="fgmres">
```

```
      <print_level>0</print_level>
      <max_iter>100</max_iter>
      <tol>0.05</tol>
      <fail_max_iters>0</fail_max_iters>
    </schur_solver>
   </pc_left>
  </default_linear_solver>
```

Chapter 9

FEBio Plugins

As of version 2.0 FEBio supports plugins. Plugins are dynamic libraries that extend the capabilities of FEBio at runtime without the need to recompile the entire source code. This offers the user a powerful mechanism for extending the default feature set of FEBio with little effort. In addition, the development of the plugin is independent of the FEBio source code, which implies that upgrading to a newer version of FEBio will not require a recompilation of the plugin[1]. The *FEBio Developer's Manual* explains in detail how to create these plugins. In this section we outline how to use the plugins with FEBio. Using plugins, users can create custom materials, boundary conditions, loads, output variables, etc. See the developer's manual for more information on what plugins can do.

9.1 Using Plugins

A plugin is compiled into a dynamic library (dll or dylib) or shared object (so) and containes the compiled code of the library. In order to use this plugin, you must add the path to and name of the plugin file in the FEBio configuration file (see Chapter 8 for a discussion of the configuration file). For each plugin, an *import* item has to be added in this configuration file. For example,

```
<import>myplugin.dll</import>
```

You may need to add the full path to the plugin if FEBio has problems locating the plugin.

```
<import>C:\path\to\my\plugins\myplugin.dll</import>
```

When FEBio starts, it will first load all the plugins that are defined in the configuration file before it reads the input file. This way, sections in the input file that require the plugin's capabilities will already be available for use.

An alternative way for loading a plugin is using the **-import** command line option.

```
>febio -i input.feb -import myplugin.dll
```

In this example, FEBio will look for the file *myplugin.dll* in the current working directory. If the plugin file is located in a different folder than the current working directory, you must prepend the relative or absolute path to the file. Note that if the path contains spaces, you need to wrap it in quotes.

```
>febio -i input.feb -import "C:\path\to\my custom plugin\myplugin.dll"
```

[1] When upgrading to a newer version of FEBio, it may be necessary to recompile the plugin if the plugin interface was changed. As long as the plugin remains compatible with the new interface, no code changes are required.

9.2 Error Messages

If FEBio cannot find a plugin it will print an error message. There are several reasons why a plugin fails to load. Below is a list of possible error messages and some actions that can be taken to prevent the error.

- *"Failed to load the file"*: Most likely FEBio cannot find the plugin file specified in the configuration file. Make sure that the file name including the path is correct and that there are no spaces at the start or end of the import tag's value string.

- *"Required plugin function PluginNumClasses not found"*: The plugin is missing a required function that FEBio needs to communicate with the plugin. Notify the developer of the plugin to fix this.

- *"Required plugin function PluginGetFactory not found"*: The plugin is missing a required function that FEBio needs to communicate with the plugin. Notify the developer of the plugin to fix this.

- *"Invalid number of classes returned by PluginNumClasses":* There was a problem with the plugin's innitialization. Notify the developer of the plugin to fix this.

- *"Required plugin function GetSDKVersion not found"*: The plugin is missing a required function that FEBio needs to communicate with the plugin. Notify the developer of the plugin to fix this.

- *"Invalid SDK version"*: The plugin was compiled with a version of the SDK that is not compatible with the FEBio version. This most likely means that the plugin must be rebuilt with a newer version of the SDK.

Appendix A

Heterogeneous model parameters

Many model parameters can be made dependent on the reference coordinates. This is useful, for instance, for defining inhomogeneous materials. There are two mechanisms for creating heterogeneous parameters: a mathematical expression, or a map.

For mathematical expressions, add the type=”math” attribute to the parameter’s definition. The value of the parameter tag can then be any mathematical expression. The upper case letters X, Y, Z, are used to denote material coordinates. The algebraic operators +, -, *, /, ^ are supported, as well as a list of functions listed in Appendix C.

```
<material id="1" name="my_material" type="neo-Hookean">
  <E type="math">X+Y+Z</E>
  <v>0.3</v>
</material>
```

For mapped parameters, use the attribute type=”map”. In this case, the value of the parameter is the name of the map that is defined in the MeshData section.

```
<material id="1" name="my_material" type="neo-Hookean">
  <E type="map">map_E</E>
  <v>0.3</v>
</material>
```

It is also possible to use maps in mathematical expressions.

```
<material id="1" name="my_material" type="neo-Hookean">
  <E type="math">5.0*map_E</E>
  <v>0.3</v>
</material>
```

Appendix B

Referencing Parameters

This appendix details how that model parameters can be referenced in the FEBio input files. This is used to

- write model parameters to the output file.
- reference model parameters in the parameter optimization input file.

The general format follows the following rule:

```
fem.property.property...property.parameter.component
```

Properties and parameters are referenced by tags separated by a periods. The first tag must be the *fem* tag, which serves as the name of the model. (In future version this name can be user defined, but for now is fixed). Next, the name of a model property must follow. The following properties are currently defined:

- **material**: references a material, defined in the *Material* section.
- **bc_fixed**: references a fixed bc, defined in the *Boundary* section.
- **bc_prescribed**: references a prescribed bc, defined in the *Boundary* section.
- **nodal_load**: references a nodal load, defined in the *Loads* section.
- **surface_load**: references a surface load, defined in the *Loads* section.
- **body_load**: references a body load, define in the *Loads* section.
- **rigid_body**: references a rigid body. Rigid bodies are defined implicitly via rigid materials.

All of these properties define arrays. A specific property can be referenced via square brackets. For instance, to reference the first material in the model, do this

```
fem.material[0]
```

Alternatively, a property can also be reference by name or by ID. In either case, use round brackets. For instance, to reference by ID, do

```
fem.material(1)
```

The ID refers to the “id” attribute that can be specified for most model components. To reference by name,

```
fem.material('MyMaterial')
```

Note the single quotes around the material name. The name is defined via the “name” attribute.

Note that rigid bodies can only be referenced via their material name.

```
fem.rigidbody('MyRigidMaterial')
```

Each property can have a list of parameters and sub-properties. To reference a parameter, just end the reference string with the name of the parameter. For example,

```
fem.material[0].E
```

Sub properties are referenced similarly. For example, assume that the first material is a biphasic material that defines the solid property.

```
fem.material[0].solid.E
```

If the parameter itself is an array, a specific item in the array is referenced using square brackets. For example, for an EFD-neo Hookean material,

```
fem.material[0].ksi[0]
```

In cases where the model parameter does not define a scalar it is possible to reference the components of the parameter. For instance, for a vec3 parameter,

```
fem.body_load[0].force.x
```

Nodal positions can also be referenced using the *mesh* property.

```
fem.mesh.node[0].position.x
```

Element data can also be accessed.

```
fem.mesh.elem[0].var('stress').xx
```

Appendix C

Math Expression

Many model parameters can be defined via mathematical expression. This appendix documents the syntax of this capability.

C.1 Functions

The following functions are currently supported.

sin(x) The sine function.

cos(x) The cosine function

tan(x) The tangent function

csc(x) The cosecans function

sec(x) The secans function

cot(x) The cotangent function

acos(x) The arccosine function

asin(x) The arcsine function

cosh(x) The hyperbolic cosine function

sinh(x) The hyperbolic sine function

tanh(x) The hyperbolic tangent function

ln(x) The natural logarithm

log(x) The logarithm with base 10

exp(x) The exponential function

sqrt(x) The square root function

abs(x) The absolute value function

sgn(x) The sign function

H(x) The Heaviside function (x = 0.5 at zero)

step(x) The right-continuous unit step function

J0(x) Bessel function of the first kind, order 0

J1(x) Bessel function of the first kind, order 1

Jn(x,n) Bessel function of the first kind, order *n*

Y0(x) Bessel function of the second kind, order 0

Y1(x) Bessel function of the second kind, order 1

Yn(x,n) Bessel function of the second kind, order *n*

sinc(x) The *sinc* function (i.e. sin(x)/x)

fac(n) The factorial of *n*

erf(x) The *error* function

erfc(x) The complementary error function (erfc(x) = 1 - erf(x))

tgamma(x) The *Gamma* function

atan2(x,y) The two-parameter arctangent function

pow(x,y) The y-th power of x

Tn(n,x) The Chebyshev polynomial of order *n*

binomial(n,m) The binomial of (n,m)

max(x1,...,xn) Returns the maximum value of the values listed

min(x1,...,xn) Returns the minimum value of the values listed

avg(x1,...,xn) Returns the average value of the values listed

C.2 Constants

The following predefined constants are supported:

pi The value of pi (= 3.1415926535897932385)

e The value of exp(1) (= 2.7182818284590452354)

gamma The Euler-Mascheroni constant (= 0.57721566490153286061)

inf A very large number (= 1e308)

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