

*Version 2.3*

**Theory Manual**

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# Introduction

## Overview of FEBio

FEBio is an implicit, nonlinear finite element solver that is specifically designed for applications in biomechanics. It offers analyses, constitutive models and boundary conditions that are relevant for this particular field. This section describes briefly the available features of FEBio. A more detailed overview of features can be found in the [User’s Manual](http://help.mrl.sci.utah.edu/help/index.jsp).

FEBio supports two analysis types, namely *quasi-static* and *quasi-static poroelastic*. In a *quasi-static* analysis the (quasi-) static response of the system is sought; inertial terms are ignored. In a *quasi-static poroelastic* analysis a coupled solid-fluid problem is solved. The latter analysis type is useful for modeling tissues that have high water content and the explicit modeling of fluid movement relative to the solid phase is important.

Several nonlinear constitutive models are available to allow the user to model the often complicated biological tissue behavior. Several isotropic constitutive models are supported such as Neo-Hookean, Mooney-Rivlin, Veronda-Westmann, Arruda-Boyce and Ogden. These models have a nonlinear stress-strain response. In addition to the isotropic models, there are several anisotropic models available. These materials show anisotropic behavior in at least one preferred direction and are useful for modeling biological tissues such as tendons, muscles and other tissues that contain fibers. FEBio also contains a *rigid body* material model, which can be used to model rigid structures whose deformation is negligible compared to the deformable geometry.

Biological tissues can interact in very complicated ways. Therefore FEBio supports a wide range of boundary conditions to model these interactions. These include prescribed displacements, nodal forces, and pressure forces. Deformable models can also be connected to rigid bodies so that the user can model prescribed rotations and torques. Rigid bodies can be connected with rigid joints. Even more complicated interactions can be modeled using FEBio’s contact interfaces. The user can choose between different types of contact interfaces, such as sliding interfaces, tied interfaces and rigid wall interfaces. A sliding interface is defined between two surfaces that are allowed to separate and slide across each other but are not allowed to penetrate. The rigid wall interface is also similar to the sliding interface, except that one of the contacting surfaces is a movable rigid wall. As of version 1.2, there is an implementation of a sliding interface that allows for fluid flow crossing the contact interface. The tied interface is similar to the sliding interface, but in this case, the surfaces are not allowed to slide or separate. In addition, the user may specify a body force which can be used to model the effects of gravity or base acceleration.

## About this document

This document is a part of a set of three manuals that accompany FEBio: the *[User’s Manual](http://help.mrl.sci.utah.edu/help/index.jsp)*[,](http://help.mrl.sci.utah.edu/help/index.jsp) describing how to use FEBio, the [online](http://febiodoc.sci.utah.edu/doxygen/) code documentation for users who wish to modify or add features to the code, and this manual, which describes the theory behind most of the FEBio algorithms.

The purpose of this manual is to provide theoretical background on many of the algorithms that are implemented in FEBio. In this way the user can develop a better understanding of how the program works and how it can be used to create well defined biomechanical simulations. The authors have tried to be as detailed as possible to make the text coherent and comprehensible, but due to the complexity of some of the topics, some descriptions only skim the surface. Many of the theoretical ideas discussed in this manual can and have filled entire bookshelves. The explanations contained herein should be sufficient to give the reader a basic understanding of the theoretical developments. References to textbooks and the primary literature are provided for further reading.

Chapter 2 starts with a brief overview of some of the important concepts in continuum mechanics. Readers who are already familiar with this field can skip this chapter, although the material may be useful to get familiar with the notation and terminology used in this manual.

Chapter 3 describes the nonlinear finite element method. It also explains the Newton-Raphson method, which is the basis for most implementations of the nonlinear finite element method. A more specialized version of this algorithm, the BFGS method, is described as well since it is used in FEBio.

In Chapter 4 the different element types that are available in FEBio are described in detail. FEBio currently supports 3D solid elements, such as the linear hexahedral, pentahedral and tetrahedral elements, as well as quadrilateral and triangular shell elements.

Chapter 5 contains a detailed description of the material models in FEBio. Most of these models are based on hyperelasticity, which is introduced in chapter 2. Several transversely isotropic materials are described as well. This also discusses the biphasic material and its implementation in FEBio.

Chapter 6 describes the basics of the theory of contact and coupling. In FEBio the user can connect the different parts of the geometry in a variety of ways. There are rigid interfaces where a deformable model is attached to a rigid model, rigid joints where two or more rigid bodies connect, and sliding interfaces where two surfaces are allowed to separate and slide across each other but are not allowed to penetrate. The various contact and coupling algorithms are discussed as well together with their implementation in FEBio.

# Continuum Mechanics

This chapter contains an overview of some of the important concepts from continuum mechanics and establishes some of the notation and terminology that will be used in the rest of this document. The section begins by introducing the important concepts of deformation, stress and strain. Next the concept of hyperelasticity is discussed. Finally the concept of virtual work is discussed. This concept will be used later to derive the nonlinear finite element equations. For a more thorough introduction to the mathematics needed for continuum mechanics, the user can consult [[1](#_ENREF_1)].

## Vectors and Tensors

It is assumed that the reader is familiar with the concepts of vectors and tensors. This section summarizes the notation and some useful relations that will be used throughout the manual.

Vectors are denoted by small, bold letters, e.g. **v**. Their components will be denoted by **, where, unless otherwise stated, Latin under scripts such as *i* or *I* will range from 1 to 3. In matrix form a vector will be represented as a column vector and its transpose as a row vector:

.

The following products are defined between vectors. Assume **u**, **v** are vectors. Also note that the Einstein summation convention is used throughout this manual [[2](#_ENREF_2)].

The *dot* or *scalar product*:

.

The *cross product*:

.

The *vector* *outer product*:

.

Note that vectors are also known as first order tensors. Scalars are known as zero order tensors. The outer product, defined by equation , is a second order tensor.

Second order tensors are denoted by bold, capital letters, e.g. **A**. Some exceptions will be made to remain consistent with the literature. For instance, the Cauchy stress tensor is denoted by . However, the nature of the objects will always be clear from the context. The following operations on tensors are defined. Assume **A** and **B** are second-order tensors.

The *double contraction* or *tensor inner product* is defined as:

.

The *trace* is defined as:

.

Here **1** is the second order identity tensor with components .

In general the components of tensors will change under a change of coordinate system. Nevertheless, certain intrinsic quantities associated with them will remain invariant under such a transformation. The scalar product between two vectors is such an example. The double contraction between two second-order tensors is another example. The following set of invariants for second-order tensors is commonly used:



A tensor **S** is called symmetric if it is equal to its transpose:

.

A tensor **W** is called anti-symmetric if it is equal to the negative of its transpose:

.

Any second order tensor **A** can be written as the sum of a symmetric tensor **S** and an anti-symmetric tensor **W**:

,

where

.

Also note that for any tensor **B** the following holds:

.

With any anti-symmetric tensor a vector **w** can be associated such that,

,

where the second order tensor  is defined as,

.

A second order **Q** tensor is called *orthogonal* if .

In the implementation of the FE method it is often convenient to write symmetric second-order tensors using *Voigt notation*. In this notation the components of a 2nd order symmetric tensor **A** are arranged as a column vector:

.

Higher order tensors will be denoted by bold, capital, script symbols, e.g. . An example of a third-order tensor is the *permutation tensor *, whose components are 1 for an even permutation of , -1 for an odd permutation of  and zero otherwise. The permutation symbol is useful for expressing the cross-product of two vectors in index notation:

.

An example of a fourth order tensor is the elasticity tensor  which, in linear elasticity theory, relates the small strain tensor  and the Cauchy stress tensor .

Higher order tensors can be constructed from second order tensors in a similar way as second order tensors can be constructed from vectors. If  and  are second order tensors, then the following fourth order tensors can be defind by requiring that the following must hold for any second order tensor :

,

,

,

.

The Cartesian component forms of the operators , ,  and  are defined as follows:

,

,

,

.

The fourth order identity tensors are defined as:



where  and . The components are given by:



## The Directional Derivative

In later sections the nonlinear finite element method will be formulated. Anticipating an iterative solution method to solve the nonlinear equations, it will be necessary to linearize the quantities involved. This linearization process will utilize a construction called the *directional derivative* [[1](#_ENREF_1)].

The directional derivative of a function  is defined as follows:

.

The quantity **x** may be a scalar, a vector or even a vector of unknown functions. For instance, consider a scalar function , where **x** is the position vector in . In this case the directional derivative is given by:



Here, the symbol (“del”) depicts the gradient operator.

The linearization of a function implies that it is approximated by a linear function. Using the directional derivative, a function *f* can be linearized as follows:

.

The directional derivative obeys the usual properties for derivatives.

(a) *sum rule*:If , then

.

(b) *product rule*: If , then

.

(c) *chain rule*: If , then

.

## Deformation, Strain and Stress

### The deformation gradient tensor

Consider the deformation of an object from an initial or *reference configuration* to a deformed or *current configuration*. The location of the material particles in the reference configuration are denoted by **X** and are known as the *material coordinates.* Their location in the current configuration is denoted by **x** and known as the *spatial coordinates*. The *deformation* *map* , which is a mapping from to, maps the coordinates of a material point to the spatial configuration:

.



Figure 2‑1. The deformation map

The displacement map **u** is defined as the difference between the spatial and material coordinates:

.

The *deformation gradient* is defined as

.

The deformation gradient relates an infinitesimal vector in the reference configuration  to the corresponding vector in the current configuration:

.

The determinant of the deformation tensor  gives the volume change, or equivalently the change in density:

.

Here  is the density in the reference configuration and  is the current density.

When dealing with incompressible and nearly incompressible materials it will prove useful to separate the volumetric and the deviatoric (distortional) components of the deformation gradient. Such a separation must ensure that the deviatoric part of the deformation gradient, namely , does not produce any change in volume. Noting that the determinant of the deformation gradient gives the volume ratio, the determinant of  must therefore satisfy,

.

This condition can be achieved by choosing  as,

.

Using the polar decomposition of a second order tensor, the deformation gradient can be written as a product of a positive definite symmetric tensor  **(or )** and a proper orthogonal tensor **R**:

.

is called the *left* *stretch tensor*,  is called the *right stretch tensor* and the orthogonal tensor is called the *rotation*.

### Strain

The *right Cauchy-Green deformation tensor* is defined as follows:

.

This tensor is an example of a *material tensor* and is a function of the material coordinates **X**. The *left Cauchy-Green deformation tensor* is defined as follows:

.

This tensor is an example of a *spatial tensor* and is a function of the spatial coordinates **x**. The implementation of the updated Lagrangian finite element method used by FEBio is described in the spatial configuration.

The left and right deformation tensors can also be split into volumetric and deviatoric components. With the use of, the deviatoric deformation tensors are:



The deformation tensors defined above are not good candidates for strain measures since in the absence of strain they become the identity tensor . However, they can be used to define strain measures. The *Green-Lagrange strain tensor* is defined as:

.

This tensor is a material tensor. Its spatial equivalent is known as the *Almansi strain tensor* and is defined as:

.

In the limit of small displacement gradients, the components of both strain tensors are identical, resulting in the *small strain tensor* or *infinitesimal strain tensor*:

.

Note that the small strain tensor is also the linearization of the Green Lagrange strain,

.

### Stress

The traction **t** on a plane bisecting the body is given by,

,

where  is the *Cauchy stress tensor* and **n** is the outward unit normal vector to the plane. It can be shown that by the conservation of angular momentum that this tensor is symmetric () [[3](#_ENREF_3)]. The Cauchy stress tensor, a spatial tensor, is the actual physical stress, that is, the force per unit deformed area. To simplify the equations of continuum mechanics, especially when working in the material configuration, several other stress measures are often used. The *Kirchhoff stress tensor* is defined as

.

The *first Piola-Kirchhoff stress tensor* is given as

.

Note that **P**, like **F**, is not symmetric. Also, like **F**, **P** is known as a *two-point* tensor, meaning it is neither a material nor a spatial tensor. Since we have two strain tensors, one spatial and one material tensor, it would be useful to have similar stress measures. The Cauchy stress is a spatial tensor and the *second Piola-Kirchhoff (2nd PK) stress tensor*, defined as

,

is a material tensor. The inverse relations are:

.

In many practical applications it is physically relevant to separate the hydrostatic stress and the deviatoric stress  of the Cauchy stress tensor:

.

Here, the pressure is defined as . Note that the deviatoric Cauchy stress tensor satisfies .

The directional derivative of the 2nd PK stress tensor needs to be calculated for the linearization of the finite element equations. For a hyperelastic material, a linear relationship between the directional derivative of and the linearized strain  can be obtained:

.

Here,  is a fourth-order tensor known as the *material elasticity tensor*. Its components are given by,

,

where  is the strain-energy density function for the hyperelastic material. The spatial equivalent – the *spatial elasticity tensor* – can be obtained by,

.

## Hyperelasticity

When the constitutive behavior is only a function of the current state of deformation, the material is *elastic*. In the special case when the work done by the stresses during a deformation is only dependent on the initial state and the final state, the material is termed *hyperelastic* and its behavior is path-independent. As a consequence of the path-independence a *strain energy function* per unit undeformed volume can be defined as the work done by the stresses from the initial to the final configuration:

.

The rate of change of the potential is then given by

.

Or alternatively,

.

Comparing with reveals that

.

This general constitutive equation can be further simplified by observing that, as a consequence of the objectivity requirement, may only depend on **F** through the stretch tensor **U** and must be independent of the rotation component **R**. For convenience, however, is often expressed as a function of **.** Noting that  is work conjugate to the second Piola-Kirchhoff stress **S**, establishes the following general relationships for hyperelastic materials:

.

### Isotropic Hyperelasticity

The hyperelastic constitutive equations discussed so far are unrestricted in their application. Isotropic material symmetry is defined by requiring the constitutive behavior to be independent of the material axis chosen and, consequently,  must only be a function of the invariants of **C**,

,

where the invariants of **C** are defined here as,

.

As a result of the isotropic restriction, the second Piola-Kirchhoff stress tensor can be written as,

.

The second order tensors formed by the derivatives of the invariants with respect to **C** can be evaluated as follows:

.

Introducing expressions into equation enables the second Piola-Kirchhoff stress to be evaluated as,

,

where , , and .

The Cauchy stresses can now be obtained from the second Piola-Kirchhoff stresses by using :

.

Note that in this equation , , and  still involve derivatives with respect to the invariants of **C**. However, since the invariants of **b** are identical to those of **C**, the quantities,  and  may also be considered to be the derivatives with respect to the invariants of **b**.

### Isotropic Elasticity in Principal Directions

For isotropic materials, the principal directions of the strain and stress tensors are the same. Let the eigenvalues of  be denoted by  (), then the strain energy density may be given as a function of these eigenvalues, . To derive the expression for the stress, recognize that

,

where the  are the eigenvectors of . It follows that the second Piola-Kirchhoff stress may be represented as

,

where

.

To evaluate the material elasticity tensor, recognize that

,

where  form a permutation over . Then it can be shown that the material elasticity tensor is given by



When eigenvalues coincide, L’Hospital’s rule may be used to evalue the coefficient in the last term,

.

The double summations in are arranged such that the summands represent fourth-order tensors with major and minor symmetries.

In the spatial frame, the Cauchy stress is given by

.

where

,

and  are the eigenvectors of . The principal normal stresses are

.

The spatial elasticity tensor is given by



### Nearly-Incompressible Hyperelasticity

A material is considered incompressible if it shows no change in volume during deformation, or otherwise stated, if  holds throughout the entire body. It can be shown [[1](#_ENREF_1)] that if the material is incompressible the hyperelastic constitutive equation becomes

,

where is the deviatoric strain energy function and *p* is the hydrostatic pressure. The presence of *J* may seem unnecessary, but retaining *J* has the advantage that equation remains valid in the nearly incompressible case. Further, in practical terms, a finite element analysis rarely enforces  in a pointwise manner, and hence its retention may be important for the evaluation of stresses.

The process of defining constitutive equations in the case of nearly incompressible hyperelasticity is simplified by adding a volumetric energy component  to the distortional component :

.

The second Piola-Kirchhoff tensor for a material defined by is obtained in the standard manner with the help of equation .



where the pressure *p* is defined as

.

An example for *U* that will be used later in the definition of the constitutive models is

.

The parameter  will be used later as a penalty factor that will enforce the (nearly-) incompressible constraint. However,  can represent a true material coefficient, namely the bulk modulus, for a compressible material that happens to have a hyperelastic strain energy function in the form of . In the case where the dilatational energy is given by , the pressure is

.

Equation can be further developed by applying the chain rule to the first term:

,

where the *fictitious second Piola-Kirchoff* tensor [[4](#_ENREF_4)] is defined by,

,

and Dev is the deviator operator in the reference frame:

.

The Cauchy stress can then be obtained from equation 3:

.

where

.

### Transversely Isotropic Hyperelasticity

Transverse isotropy can be introduced by adding a vector field representing the material preferred direction explicitly into the strain energy [[5](#_ENREF_5)]. We require that the strain energy depends on a unit vector field , which describes the local fiber direction in the undeformed configuration. When the material undergoes deformation, the vector  may be described by a unit vector field . In general, the fibers will also undergo length change. The fiber stretch, , can be determined in terms of the deformation gradient and the fiber direction in the undeformed configuration,

.

Also, since  is a unit vector,

.

The strain energy function for a transversely isotropic material,  is an isotropic function of  and . It can be shown [[3](#_ENREF_3)] that the following set of invariants are sufficient to describe the material fully:





The strain energy function can be written in terms of these invariants such that

.

The second Piola-Kirchhoff can now be obtained in the standard manner:

.

In the transversely isotropic constitutive models described in Chapter 5 it is further assumed that the strain energy function can be split into the following terms:

.

The strain energy function  represents the material response of the isotropic ground substance matrix,  represents the contribution from the fiber family (e.g. collagen), and  is the contribution from interactions between the fibers and matrix. The form generalizes many constitutive equations that have been successfully used in the past to describe biological soft tissues e.g. [[6-8](#_ENREF_6)]. While this relation represents a large simplification when compared to the general case, it also embodies almost all of the material behavior that one would expect from transversely isotropic, large deformation matrix-fiber composites.

## Biphasic Material

Biphasic materials may be used to model deformable porous media. A biphasic material represents a mixture of a porous permeable solid and an interstitial fluid. Each constituent is intrinsically incompressible, but the mixture may change volume as interstitial fluid is exchanged with the pore space of the solid. Biphasic materials require the explicit modeling of fluid that permeates the solid. The biphasic material model is useful to simulate materials that show flow-dependent viscoelastic behavior resulting from the frictional interactions of the fluid and solid. Several biological materials such as cartilage can be described more accurately this way.

### Governing Equations

Consider a mixture consisting of a solid constituent and a fluid constituent. Both constituents are considered to be intrinsically incompressible, but the mixture can change volume when fluid enters or leaves the porous solid matrix [[9](#_ENREF_9), [10](#_ENREF_10)]. According to the kinematics of the continuum [[11](#_ENREF_11)], each constituent  of a mixture ( for the solid and  for the fluid) has a separate motion  which places particles of each mixture constituent, originally located at , in the current configuration  according to

.

For the purpose of finite element analyses, the motion of the solid matrix, , is of particular interest.

The governing equations that enter into the statement of virtual work are the conservation of linear momentum and the conservation of mass, for the mixture as a whole. Under quasi-static conditions, the conservation of momentum reduces to

,

where  is the Cauchy stress for the mixture,  is the mixture density and  is the external mixture body force per mass. Since the mixture is porous, this stress may also be written as

,

where  is the fluid pressure and  is the effective or extra stress, resulting from the deformation of the solid matrix. Conservation of mass for the mixture requires that

,

where  is the solid matrix velocity and  is the flux of the fluid relative to the solid matrix. Let the solid matrix displacement be denoted by , then .

To relate the relative fluid flux  to the fluid pressure and solid deformation, it is necessary to employ the equation of conservation of linear momentum for the fluid,

,

where  is the solid matrix porosity,  is the apparent fluid density and  is the true fluid density,  is the external body force per mass acting on the fluid, and  is the momentum exchange between the solid and fluid constituents, typically representing the frictional interaction between these constituents. This equation neglects the viscous stress of the fluid in comparison to . The most common constitutive relation is , where the second order, symmetric tensor  is the hydraulic permeability of the mixture. When combined with Eq., it produces

,

which is equivalent to Darcy’s law. In general,  may be a function of the deformation.

## Biphasic-Solute Material

A biphasic-solute material is an extension of the biphasic material model that also includes transport and mechano-chemical effects of a neutral solute. Transport of a solute in a porous medium includes diffusion, resulting from gradients in the solute concentration, and convection of the solute by the solvent, as a result of fluid pressure gradients. Mechano-chemical effects describe phenomena such as osmotic pressurization and swelling.

### Governing Equations

The governing equations adopted in this finite element implementation of neutral solute transport in deformable porous media are based on the framework of mixture theory [[11](#_ENREF_11), [12](#_ENREF_12)]. A single solute is considered in this presentation for notational simplicity, though the extension of equations to multiple solutes is straightforward. Various forms of the governing equations have been presented in the prior literature [[13](#_ENREF_13), [14](#_ENREF_14)], though a presentation that incorporates all the desired features of this implementation has not been reported previously and is thus detailed here.

The fundamental modeling assumptions adopted in this treatment are quasi-static conditions for momentum balance (negligible effects of inertia), intrinsic incompressibility of all constituents (invariant true densities), isothermal conditions, negligible volume fraction of solute relative to the solid and solvent, and negligible effects of solute and solvent viscosities (friction within constituents) relative to frictional interactions between constituents. These assumptions are often made in studies of biological tissues and cells. External body forces and chemical reactions are not considered.

The three constituents of the mixture are the porous-permeable solid matrix (), the solvent (), and the solute (). The motion of the solid matrix is described by the displacement vector , the pressure of the interstitial fluid (solvent+solute) is , and the solute concentration (on a solution-volume basis) is . The total (or mixture) stress may be described by the Cauchy stress tensor , where  is the identity tensor and  is the stress arising from the strain in the porous solid matrix. Because it is porous, the solid matrix is compressible since the volume of pores changes as interstitial fluid enters or leaves the matrix. Under the conditions outlined above, the balance of linear momentum for the mixture reduces to

.

Similarly, the equations of balance of linear momentum for the solvent and solute are given by



where  is the apparent density (mass of  per volume of the mixture),  is the mechano-chemical potential and  is the velocity of constituent .  is the diffusive drag tensor between constituents  and  representing momentum exchange via frictional interactions, which satisfies . An important feature of these relations is the incorporation of momentum exchange term between the solute and solid matrix, , which is often neglected in other treatments but plays an important role for describing solid-solute interactions [[13](#_ENREF_13), [15](#_ENREF_15), [16](#_ENREF_16)]. These momentum equations show that the driving force for the transport of solvent or solute is the gradient in its mechano-chemical potential, which is resisted by frictional interactions with other constituents.

The mechano-chemical potential is the sum of the mechanical and chemical potentials. The chemical potential  of  represents the rate at which the mixture free energy changes with increasing mass of . The mechanical potential represents the rate at which the mixture free energy density changes with increasing volumetric strain of . In a mixture of intrinsically incompressible constituents, where the volumetric strain is idealized to be zero, this potential is given by , where  is the true density of  (mass of  per volume of ), which is invariant for incompressible constituents, and  is some arbitrarily set reference pressure (e.g., ambient pressure).

From classical physical chemistry, the general form of a constitutive relation for the chemical potential is  [[17](#_ENREF_17)], where  is the universal gas constant,  is the absolute temperature,  is the molecular weight (invariant) and  is the activity of constituent  (a non-dimensional quantity);  is the chemical potential at some arbitrary reference state, at a given temperature. For solutes, physical chemistry treatments let , where  is the solute concentration in some standard reference state (an invariant, typically ), and  is the non-dimensional activity coefficient, which generally depends on the current state (e.g., concentration) but reduces to unity under the assumption of ideal physico-chemical behavior [[17](#_ENREF_17)]. Since this representation is strictly valid for free solutions only, whereas solutes may be partially excluded from some of the interstitial space of a porous solid matrix, Mauck et al. [[13](#_ENREF_13)] extended this representation of the solute activity to let , where the solubility  represents the fraction of the pore space which is accessible to the solute (). In this extended form, it becomes clear that even under ideal behavior (), the solute activity may be affected by the solubility. Indeed, for neutral solutes, the solubility also represents the partition coefficient of the solute between the tissue and external bath [[18](#_ENREF_18), [19](#_ENREF_19)].

When accounting for the fact that the solute volume fraction is negligible compared to the solvent volume fraction [[17](#_ENREF_17), [20](#_ENREF_20)], the general expressions for  and  take the form



where  is the osmotic coefficient (a non-dimensional function of the state), which deviates from unity under non-ideal physico-chemical behavior. Therefore, a complete description of the physico-chemical state of solvent and solute requires constitutive relations for  and the effective solubility , which should generally depend on the solid matrix strain and the solute concentration.

It is also necessary to satisfy the balance of mass for each of the constituents. In the absence of chemical reactions, the statement of balance of mass for constituent  reduces to

.

The apparent density may be related to the true density via , where  is the volume fraction of  in the mixture. Due to mixture saturation (no voids), the volume fractions add up to unity. Since the volume fraction of solute is considered negligible (), it follows that . Since  of an incompressible constituent is invariant in space and time, these relations may be combined to produce the mixture balance of mass relation,

,

where  is the volumetric flux of solvent relative to the solid. The balance of mass for the solute may also be written as

,

where  is the molar flux of solute relative to the solid. This mass balance relation is obtained by recognizing that the solute apparent density (mass per mixture volume) is related to its concentration (moles per solution volume) via . Finally, it can be shown via standard arguments that the mass balance for the solid matrix reduces to

,

where  is the solid volume fraction in the reference state,  and  is the deformation gradient of the solid matrix.

Inverting the momentum balance equations in , it is now possible to relate the solvent and solute fluxes to the driving forces according to



where  is the solute diffusivity tensor in the mixture (solid+solution),  is its (isotropic) diffusivity in free solution;  is the hydraulic permeability tensor of the solution (solvent+solute) through the porous solid matrix, which depends explicitly on concentration according to

,

where  represents the hydraulic permeability tensor of the solvent through the solid matrix. The permeability and diffusivity tensors are related to the diffusive drag tensors appearing in according to



though these explicit relationships are not needed here since ,  and  may be directly specified in a particular analysis. Since the axiom of entropy inequality requires that the tensors  be positive semi-definite (see appendix of [[21](#_ENREF_21)]), it follows that  must be greater than or equal to the largest eigenvalue of . Constitutive relations are needed for these transport properties, which relate them to the solid matrix strain and solute concentration. Note that the relations in represent generalizations of Darcy’s law for fluid permeation through porous media, and Fick’s law for solute diffusion in porous media or free solution.

### Continuous Variables

In principle, the objective of the finite element analysis is to solve for the three unknowns, ,  and , using the partial differential equations that enforce mixture momentum balance in , mixture mass balance in , and solute mass balance in . The remaining solvent and solute momentum balances in , and solid mass balance in , have been reduced to relations that may be substituted into the three partial differential equations as needed. Solving these equations requires the application of suitable boundary conditions that are consistent with mass, momentum and energy balances across boundary surfaces or interfaces. When defining boundaries or interfaces on the solid matrix (the conventional approach in solid mechanics), whose outward unit normal is , mass and momentum balance relations demonstrate that the mixture traction  and normal flux components  and  must be continuous across the interface [[20](#_ENREF_20), [22](#_ENREF_22)]. Therefore, ,  and  may be prescribed as boundary conditions.

Combining momentum and energy balances across an interface also demonstrates that  and  must be continuous [[20](#_ENREF_20), [23](#_ENREF_23)], implying that these mechano-chemical potentials may be prescribed as boundary conditions. However, because of the arbitrariness of the reference states , ,  and , and the ill-conditioning of the logarithm function in the limit of small solute concentration, the mechano-chemical potentials do not represent practical choices for primary variables in a finite element implementation. An examination of also shows that continuity of these potentials across an interface does not imply continuity of the fluid pressure  or solute concentration . Therefore, pressure and concentration are also unsuitable as nodal variables in a finite element analysis and they must be replaced by alternative choices. Based on the similar reasoning presented by Sun et al. [[24](#_ENREF_24)], an examination of the expressions in shows that continuity may be enforced by using



where  is the effective fluid pressure and  is the effective solute concentration in the mixture. Note that  represents that part of the fluid pressure which does not result from osmotic effects (since the term  may be viewed as the osmotic pressure contribution to ), and  is a straightforward measure of the solute activity, since . Therefore these alternative variables have clear physical meanings.

Since the unknowns are now given by ,  and , the governing partial differential equations may be rewritten in the form



where



Constitutive equations are needed to relate , , , ,  and  to the solid matrix strain and effective solute concentration.

## Triphasic and Multiphasic Materials

Multiphasic materials represent an extension of the biphasic-solute material, where the mixture may contain a multitude of solutes. These solutes may be either electrically charged (ionized) or neutral. Similarly, the solid matrix may either carry electrical charge (a fixed charge density) or be neutral. A triphasic material is a special case of a multiphasic material, having two solutes that carry opposite charges. Triphasic and multiphasic materials may be used to model porous deformable biological tissues whose solid matrix may be charged and whose interstitial fluid may contain any number of charged or neutral solutes. When mixture constituents are electrically charged, the response of the tissue to various loading conditions may encompass a range of mechano-electrochemical phenomena, including permeation, diffusion, osmosis, streaming potentials and streaming currents. To better understand multiphasic materials, the reader is encouraged to review the descriptions of biphasic (Section 2.5) and biphasic-solute materials (Section 2.6).

### Governing Equations

In multiphasic materials the solvent is assumed to be neutral, whereas the solid and solutes may carry charge. The mixture is isothermal and all constituents are considered to be intrinsically incompressible. Since the viscosity of the fluid constituents (solvent and solutes) is considered negligible relative to the frictional interactions among constituents, the stress tensor  for the mixture includes only a contribution from the fluid pressure  and the stress  in the solid,

.

The mechano-chemical potential of the solvent is given by

,

where  is the solvent chemical potential in the solvent standard state,  is the absolute temperature,  is the true density of the solvent (which is invariant since the solvent is assumed intrinsically incompressible),  is the fluid pressure,  is the corresponding pressure in the standard state,  is the universal gas constant,  is the non-dimensional osmotic coefficient, and  is the solution volume-based concentration of solute . The summation is taken over all solutes in the mixture. The mechano-electrochemical potential of each solute is similarly given by

,

where  is the molar mass of the solute,  is its activity coefficient,  is its solubility,  is its charge number, and  is its concentration in the solute standard state;  is Faraday’s constant,  is the electrical potential of the mixture, and  is the corresponding potential in the standard state.

In these relations,  and  are functions of state that describe the deviation of the mixture from ideal physico-chemical behavior;  represents the fraction of the pore volume which may be occupied by solute . The standard state represents an arbitrary set of reference conditions for the physico-chemical state of each constituent. Therefore, the values of , , , , and , remain invariant over the entire domain of definition of an analysis. Since  and  appear together as a ratio, they may be combined into a single material function, , called the effective solubility.

In multiphasic mixtures, it is also assumed that electroneutrality is satisfied at every point in the continuum. Therefore, the net electrical charge summed over all constituents must reduce to zero, and no net charge accumulation may occur at any time. Denoting the fixed charge density of the solid by  (moles of equivalent charge per solution volume), and recognizing that the solvent is always considered neutral, the electroneutrality condition may be written as

.

This condition represents a constraint on a mixture of charged constituents. If none of the constituents are charged ( and  for all ), the constraint disappears.

Each constituent of the mixture must satisfy the axiom of mass balance. In the absence of chemical reactions involving constituent , its mass balance equation is

,

where  is the apparent density and  is the velocity of that constituent. For solutes, the apparent density is related to the concentration according to , where  is the volume fraction of the solid. When the solute volume fractions are negligible, it follows that , where  is the solvent volume fraction. The molar flux of the solute relative to the solid is given by , where  is the solute velocity. Using these relations, the mass balance relation for the solute may be rewritten as

,

where  represents the material time derivative in the spatial frame, following the solid; , where  is the deformation gradient of the solid. This form of the mass balance for the solute is convenient for a finite element formulation where the mesh is defined on the solid matrix.

The volume flux of solvent relative to the solid is given by , where  is the solvent velocity. When solute volume fractions are negligible, the mass balance equation for the mixture reduces to .

Finally, the mass balance for the solid may be reduced to the form , which may be integrated to produce the algebraic relation , where  is the solid volume fraction in the stress-free reference state of the solid.

Differentiating the electroneutrality condition in using the material time derivative following the solid, and substituting the mass balance relations into the resulting expressions, produces a constraint on the solute fluxes:

.

Recognizing that  is the current density in the mixture, with  representing Faraday’s constant, the relation of reduces to one of the Maxwell’s equation, , in the special case when there can be no charge accumulation (electroneutrality).

As described in Section 2.6.2, the fluid pressure  and solute concentrations  are not continuous across boundaries of a mixture, whereas  and ’s for the solutes do satisfy continuity. Therefore, in a finite element implementation, the following continuous variables are used as nodal degrees of freedom:

,

which represents the effective fluid pressure, and

,

which represents the effective solute concentration. In the last expression,  is the partition coefficient of the solute, which is related to the effective solubility and electric potential according to

.

Physically, since  is the osmotic (chemical) contribution to the fluid pressure,  may be interpreted as that part of the total (mechano-chemical) fluid pressure which does not result from osmotic effects; thus, it is the mechanical contribution to . Similarly, the effective solute concentration  represents the true contribution of the molar solute content to its electrochemical potential.

When using these variables instead of mechano-electrochemical potentials, the momentum equations for the solvent and solutes may be inverted to produce the following flux relations:

,

and

,

where



is the effective hydraulic permeability of the solution (solvent+solutes) in the mixture. The momentum equation for the mixture is

.

## Mixture of Solids

A solid material may consist of a heterogeneous mixture of various solid constituents that are constrained to move together. If each constituent is denoted by the superscript , a constrained mixture satisfies  for all , where  is the velocity of the solid mixture. For example, a fiber-reinforced material may consist of a mixture of fibers and a ground matrix. In general, the constitutive relation for such a constrained mixture of solids may be a complex function of the mass fraction of each constituent as well as the ultrastructure of the constituents and their mutual interactions. The mass fraction of each constituent may be represented by the apparent density , which is the ratio of the mass of  to the volume of the mixture in the reference configuration, in an elemental region. In the framework of hyperelasticity, the general representation for the strain energy density for such a solid mixture may have the form

,

where  is the deformation gradient of constituent  and  is the number of solid constituents in the mixture. Though the solid constituents are constrained to move together, their deformation gradients are not necessarily the same, depending on how the various solid constituents of a constrained mixture were assembled [[25](#_ENREF_25)].

With no loss of generality, it may be assumed that the strain energy density of the mixture is the summation of the strain energy densities of all the constituents,

,

where  is the strain energy density of constituent .

Now, *as a special case*, we may assume that the simplest form of the constitutive relation for a mixture of constrained solids is

.

This special form assumes that there are no explicit dependencies among the various solid constituents of the mixture. Thus,  depends only on the deformation gradient and mass content of .

Furthermore, if we assume that  for all  (implying no residual stresses in the solid mixture), then the general form for  further reduces to

.

Consequently, the stress tensor for the mixture becomes

.

In other words, the stress in the solid mixture may be evaluated from the sum of the stresses in each mixture constituent using the same hyperelasticity relation as for a single, pure solid constituent. The fact that  also depends on  implies that the material properties appearing in the constitutive relation for  are dependent on the mass content of solid  in the mixture.

For nearly-incompressible solids, using a reasoning similar to that which led to , the uncoupled strain energy density for the solid mixture may be of the form

,

where  is the volumetric energy component,  is the distortional energy component, and  is the distortional part of the deformation gradient, as described in Section 2.4.3.

## Equilibrium Swelling

When the interstitial fluid of a porous medium contains one or more solutes, an osmotic pressure may be produced in the fluid if the osmolarity of the interstitial fluid is non-uniform, or if it is different from that of the external bathing solution surrounding the porous medium. In general, since the osmolarity of the interstitial fluid may vary over time in transient problems, the analysis of such swelling effects may be addressed using, for example, the biphasic-solute material model described in Section 2.6. However, if we are only interested in the steady-state response for such types of materials, when solvent and solute fluxes have subsided, the analysis may be simplified considerably.

The Cauchy stress tensor for a mixture of a porous solid and interstitial fluid is given by

,

where  is he fluid pressure and  is the stress in the solid matrix resulting from solid strain. When steady-state conditions are achieved, the fluid pressure  results exclusively from osmotic effects and ambient conditions (i.e., it does not depend on the loading history). Thus, in analogy to ,  where  is the mechanical pressure resulting from ambient conditions and  is the osmotic pressure resulting from the osmolarity  of the solution.

The osmotic pressure  may produce swelling of the solid matrix, which is opposed by the solid matrix stress. This becomes more apparent when considering, for example, the case of a traction-free body. The traction is given by , where  is the unit outward normal to the boundary. When , the relation of produces , clearly showing that the osmotic pressure  is balanced by the swelling solid matrix.

The interstitial osmolarity (number of moles of solute per volume of interstitial fluid) may be related to the solute and solid content according to

,

where  is the number of moles of solute per volume of the mixture in the reference configuration,  is the volume fraction of the solid in the reference configuration, and  is the relative volume of the porous solid matrix. Neither  nor  depend on the solid matrix deformation, thus provides the explicit dependence of  on . This relation shows that the osmolarity of the interstitial fluid is dependent on the relative change in volume of the solid matrix with deformation. Effectively, under equilibrium swelling conditions, the term  in represents an elastic stress and may be treated in this manner when analyzing equilibrium swelling conditions.

Since  also depends on the osmotic coefficient, if we assume that  depends on the solid strain at most via a dependence on , we may thus state generically that  under equilibrium swelling. It follows that the elasticity tensor for  is

,

where  is the elasticity tensor of .

### Perfect Osmometer

Consider a porous medium with an interstitial fluid that consists of a solvent and one or more solutes, whose boundary is permeable to the solvent but not to the solutes (e.g., a biological cell). Since solutes are trapped within such a medium,  is a constant in this type of problem. Since the boundary is permeable to the solvent,  must be continuous across the boundary. Assuming ideal physicochemical conditions, , and zero ambient pressure, this continuity requirement implies that , where is the osmolarity of the external environment. Using , it follows that

.

The reference configuration (the stress-free configuration of the solid) is achieved when  and , from which it follows that , where  is the value of  in the reference state. Therefore may also be written as

,

and this expression may be substituted into to evaluate the corresponding elasticity tensor.

A perfect osmometer is a porous material whose interstitial fluid behaves ideally and whose solid matrix exhibits negligible resistance to swelling (). In that case  and may be rearranged to yield

.

This equation is known as the Boyle-van’t Hoff relation for a perfect osmometer. It predicts that variations in the relative volume of such as medium with changes in external osmolarity  is an affine function of , with the intercept at the origin representing the solid volume fraction and the slope representing the fluid volume fraction, in the reference configuration.

FEBio implements the relation of for the purpose of modeling equilibrium swelling even when solid matrix stresses are not negligible. The name “perfect osmometer” is adopted for this model because it reproduces the Boyle-van’t Hoff response in the special case when .

### Cell Growth

The growth of cells requires the active uptake of soluble mass to provide the building blocks for various intracellular structures, such as the cytoskeleton or chromosomes, and growth contributes to the osmolarity of the intracellular space. The resulting mechano-chemical gradient drives solvent into the cell as well, contributing to its volumetric growth.

Cell growth may be modeled using the “perfect osmometer” framework by simply increasing the mass of the intracellular solid matrix and membrane-impermeant solute. This is achieved by using to model the osmotic pressure and allowing the parameters  and  (normally constant) to increase over time as a result of growth. 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  and  increase proportionally, though this is not an obligatory relationship. To ensure that the initial configuration is a stress-free reference configuration, let  in the initial state prior to growth.

### Donnan Equilibrium Swelling

Consider a porous medium whose solid matrix holds a fixed electrical charge and whose interstitial fluid consists of a solvent and two monovalent counter-ions (such as Na+ and Cl-). The boundaries of the medium are permeable to the solvent and ions. The fixed charge density is denoted by ; it is a measure of the number of fixed charges per volume of the interstitial fluid in the current configuration. This charge density may be either negative or positive, thereby producing an imbalance in the concentration of anions and cations in the interstitial fluid. To determine the osmolarity of the interstitial fluid, it is necessary to equate the mechano-chemical potential of the solvent and the mechano-electrochemical potential of the ions between the porous medium and its surrounding bath. When assuming ideal physicochemical behavior, the interstitial osmolarity (resulting from the interstitial ions) is given by

,

where  is the salt concentration in the bath. Alternatively, we note that the osmolarity of the bath is . Though this expression may be equated with , the resulting value of  is not constant in this case, since ions may transport into or out of the pore space; therefore that relation is not useful here.

However, since the number of charges fixed to the solid matrix is invariant, we may manipulate to produce a relation between the fixed charge density in the current configuration, , and the corresponding value in the reference configuration,,

.

Now the osmotic pressure resulting from the difference in osmolarity between the porous medium and its surrounding bath is given by

.

This expression may be substituted into to evaluate the corresponding elasticity tensor.

When the osmotic pressure results from an imbalance in osmolarity produced by a fixed charge density, it is called a Donnan osmotic pressure. The analysis associated with this relation is called Donnan equilibrium.

## Chemical Reactions

Chemical reactions may be incorportated into a multiphasic mixture by adding a mass supply term to the equation of mass balance,

,

Where  is the volume density of mass supply to  resulting from chemical reactions with all other mixture constitutents. Since mass must be conserved over all constituents, mass supply terms are constrained by

.

In a mixture containing a solid constituent (denoted by  ), it is conveniemt to define the mixture domain (and thus the finite element mesh) on the solid and evaluate mass fluxes of constituents relative to the solid,

.

Substituting into , the differential form of the mass balance may be rewritten as

,

Where  represents the material time derivative in the spatial frame, following the solid, , where  is the deformation gradient of the solid matrix;  is the apparent density and  is the volume density of mass supply to  normalized to the mixture volume in the reference configuration,

.

Since  is the mass of  in the current configuration per volume of the mixture in the reference configuration (an invariant quantity), this parameter represents a direct measure of the mass content of  in the mixture, which may thus be used as a state variable in a framework that accounts for chemical reactions. A distinction is now made between solid and solute species in the mixture, since they are often treated differential in an analysis.

### Solid Matrix and Solid-Bound Molecular Constituents

For constituents constrained to move with the solid (denoted generically by  and satisfying  , ), the statement of mass balance in reduces to the special form

.

This representation makes it easy to see that alterations in  can occur only as a result of chemical reactions (such as synthesis, degradation, or binding). In contrast, as seen in , alterations in  for solutes or solvent () may also occur as a result of mass transport into or out of the pore space of the solid matrix. Therefore,  is the natural choice of state variable for describing the content of solid constituents in a reactive mixture.

When multiple solid species are present, the net solid mass content may be given by  whereas the net mass supply of solid is  such that . The referential solid volume fraction, , may be evaluated from

,

where  is the true density of solid constituent  (mass of  per volume of ). According to , it follows that the solid volume fraction in the current configuration is given by . Note that  under all circumstances, while , implying that  may exceed unity when solid growth occurs. In this study, it is assumed that all mixture constituents are intrinsically incompressible, implying that

their true density is invariant.

The various constituents of the solid matrix may be electrically charged. Let  be the charge number (equivalent charge per mole) of solid constituent , then the net referential fixed charge density of the solid matrix (equivalent charge per fluid volume in the referential configuration) is given by

,

where  is the molar mass of  (an invariant quantity) and  represents the referential volume fraction of all fluid constituents (solvent + solutes) in a saturated mixture. Based on the kinematics of the continuum, the fixed charge density in the current configuration is

.

### Solutes

Solutes are denoted generically by . In chemistry solute content is often represented in units of molar concentration (moles per fluid volume). It follows that solute molar concentration  and molar supply  are related to  and  via

.

The molar flux of constituent  relative to the solid is given by

,

where it may be noted that . Combining these relations with - produces the desired form of the mass balance for the solutes,

.

This form is suitable for implementation in a finite element analysis where the mesh is defined on the solid matrix.

### Mixture with Negligible Solute Volume Fraction

The volume fraction of each constituent is given by . In a saturated mixture these volume fractions satisfy . Substituting  into , dividing across by  (invariant for intrinsically incompressible constituents), and taking the sum of the resulting expression over all constituents produces

.

This mass balance relation for the mixture expresses the fact that the mixture volume will change as a result of chemical reactions where the true density of products is different from that of reactants. Indeed, assuming that  is the same for all  would nullify the right-hand-side of based on . We now adopt the assumption that solutes occupy a negligible volume fraction of the mixture (), from which it follows that  and , where  is the volumetrix flux of solvent relative to the solid. Thus, the mixture mass balance may be reduced to

.

### Chemical Kinetics

Productions rates are described by constitutive relations which are functions of the state variables. In a biological mixture under isothermal conditions, the minimum set of state variables needed to describe reactive mixtures that include a solid matrix are: the (uniform) temperature , the solid matrix deformation gradient  (or related strain measures), and the molar content  of the various constituents. This set differs from the classical treatment of chemical kinetics in fluid mixtures by the inclusion of  and the subset of constituents bound to the solid matrix. To maintain a consistent notation in this section, solid-bound molecular species are described by their molar concentrations and molar supplies which may be related to their referential mass density and referential mass supply according to

.

Consider a general chemical reaction,

,

where  is the chemical species representing constituent ;  and  represent stoichiometric coefficients of the reactants and products, respectively. Since the molar supply of reactants and products is constrained by stoichiometry, it follows that all molar supplies  in a specific chemical reaction may be related to a production rate  according to

,

where  represents the net stoichiometric coefficient for ,

.

Thus, formulating constitutive relations for  is equivalent to providing a single relation for . When the chemical reaction is reversible,

,

the relations of - still apply but the form of  would be different.

Using the relations of , and , it follows in general that , so that the constraint of is equivalent to enforcing stoichiometry, namely,

.

Thus, properly balancing a chemical reaction satisfies this constraint.

The mixture mass balance in may now be rewritten as

,

where  and  is the molar volume of . Similarly, the solute mass balance in becomes

.

These mass balance equations reduce to those of non-reactive mixtures when .

# The Nonlinear FE Method

This chapter discusses the basic principles of the nonlinear finite element method. The chapter begins with a short introduction to the weak formulation and the principle of virtual work. Next, the important concept of linearization is discussed and applied to the principle of virtual work. Finally the Newton-Raphson procedure and its application to the nonlinear finite element method are described.

## Weak formulation for Solid Materials

Generally, the finite element formulation is established in terms of a weak form of the differential equations under consideration. In the context of solid mechanics this implies the use of the virtual work equation:

.

Here, is a virtual velocity and is the virtual rate of deformation tensor. This equation is known as the *spatial virtual work equation* since it is formulated using spatial quantities only. We can also define the *material virtual work equation* by expressing the principle of virtual work using only material quantities.

.

Here, is the body force per unit undeformed volume and is the traction vector per unit initial area.

### Linearization

Equation is the starting point for the nonlinear finite element method. It is highly nonlinear and any method attempting to solve this equation, such as the Newton-Raphson method, necessarily has to be iterative.

To linearize the finite element equations, the directional derivative of the virtual work in equation must be calculated. In an iterative procedure, the quantity  will be approximated by a trial solution . Linearization of the virtual work equation around this trial solution gives

.

The directional derivative of the virtual work will eventually lead to the definition of the stiffness matrix. In order to proceed, it is convenient to split the virtual work into an internal and external virtual work component:

,

where

,

and

.

The result is listed here without details of the derivation – see [[1](#_ENREF_1)] for details. The linearization of the internal virtual work is given by

.

Notice that this equation is symmetric in and . This symmetry will, upon discretization, yield a symmetric tangent matrix.

The external virtual work has contributions from both body forces and surface tractions. The precise form of the linearized external virtual work depends on the form of these forces. For surface tractions, normal pressure forces may be represented in FEBio. The linearized external work for this type of traction is given by



Discretization of this equation will also lead to a symmetric component of the tangent matrix.

FEBio currently supports gravity as a body force, . Since this force is independent of the geometry, the contribution to the linearized external work is zero. Another type of body force implemented in FEBio is the centrifugal force. For a body rotating with a constant angular speed , about an axis passing through the point  and directed along the unit vector , the body force is given by , where  is the vector distance from a point  to the axis of rotation,





The resulting linearized external work is given by

,

which produces a symmetric expression that will yield a symmetric matrix.

### Discretization

The basis of the finite element method is that the domain of the problem (that is, the volume of the object under consideration) is divided into smaller subunits, called *finite elements*. In the case of *isoparametric elements* it is further assumed that each element has a local coordinate system, named the *natural coordinates*, and the coordinates and shape of the element are discretized using the same functions. The discretization process is established by interpolating the geometry in terms of the coordinates  of the *nodes* that define the geometry of a finite element, and the *shape functions*:

,

where *n* is the number of nodes and are the natural coordinates. Similarly, the motion is described in terms of the current position  of the *same* particles:

.

Quantities such as displacement, velocity and virtual velocity can be discretized in a similar way.

In deriving the discretized equilibrium equations, the integrations performed over the entire volume can be written as a sum of integrations constrained to the volume of an element. For this reason, the discretized equations are defined in terms of integrations over a particular element *e*. The discretized equilibrium equations for this particular element per node is given by

,

where



The linearization of the internal virtual work can be split into a *material* and an *initial stress* component [[1](#_ENREF_1)]:



The constitutive component can be discretized as follows:

.

The term in parentheses defines the constitutive component of the tangent matrix relating node *a* to node *b* in element *e*:

.

Here, the linear strain-displacement matrix **B** relates the displacements to the small-strain tensor in Voigt Notation:

.

Or, written out completely,

.

The spatial constitutive matrix **D** is constructed from the components of the fourth-order tensor using the following table; where

|  |  |  |
| --- | --- | --- |
| **I/J** | **i/k** | **j/l** |
| 1 | 1 | 1 |
| 2 | 2 | 2 |
| 3 | 3 | 3 |
| 4 | 1 | 2 |
| 5 | 2 | 3 |
| 6 | 1 | 3 |

The initial stress component can be written as follows:

.

For the pressure component of the external virtual work, we find

,

where,



## Weak formulation for biphasic materials

A weak form of the statement conservation of linear momemtum for the quasi-static case is obtained by using Eqs. and :

,

where  is the domain of interest defined on the solid matrix,  is a virtual velocity of the solid and  is a virtual pressure of the fluid [[26](#_ENREF_26)].  is an elemental volume of . Using the divergence theorem, this expression may be rearranged as

,

where  is the virtual rate of deformation tensor,  is the total traction on the surface , and  is the component of the fluid flux normal to , with  representing the unit outward normal to .  represents an elemental area of . In this type of problem, essential boundary conditions are prescribed for  and , and natural boundary conditions are prescribed for  and . In the expression of Eq.,  represents the virtual work.

### Linearization

Since the system of equations in Eq. is highly nonlinear, its solution requires an iterative scheme such as Newton’s method. This requires the linearization of  at some trial solution , along an increment  in  and an increment  in ,

,

where  represents the directional derivative of  along . For convenience, the virtual work may be separated into its internal and external parts,

,

where

,

and

.

The evaluation of the directional derivatives can be performed following a standard approach [[1](#_ENREF_1)]. For the internal part of the virtual work, the directional derivative along  yields



where  is the fourth-order spatial elasticity tensor for the mixture and . Based on the relation of Eq., the spatial elasticity tensor may also be expanded as

,

where  is the spatial elasticity tensor for the solid matrix [[27](#_ENREF_27)]. It is related to the material elasticity tensor  via

,

where  is the deformation gradient of the solid matrix,  where  is the Lagrangian strain tensor and  is the second Piola-Kirchhoff stress tensor, related to the Cauchy stress tensor via .

Similarly,  is a fourth-order tensor that represents the spatial measure of the rate of change of permeability with strain. It is related to its material frame equivalent  via

,

where  and  is the permeability tensor in the material frame, such that . Since  and  are symmetric tensors, it follows that  and  exhibit two minor symmetries (e.g.,  and ). However, unlike the elasticity tensor, it is not necessary that these tensors exhibit major symmetry (e.g.,  in general).

The directional derivative of  along  is given by

.

Note that letting  and  in the above equations recovers the virtual work relations for nonlinear elasticity of compressible solids. The resulting simplified equation emerging from Eq. is symmetric to interchanges of  and , producing a symmetric stiffness matrix in the finite element formulation [[1](#_ENREF_1)]. However, the general relations of Eqs. and do not exhibit symmetry to interchanges of  and , implying that the finite element stiffness matrix for a solid-fluid mixture is not symmetric under general conditions.

The directional derivatives of the external virtual work  depend on the type of boundary conditions being considered. For a prescribed total normal traction , where ,

,

and



where



are covariant basis (tangent) vectors on , such that

.

For a prescribed normal effective traction , where  and  is not prescribed, then

,

and



For a prescribed normal fluid flux ,

,

and



Finally, for a prescribed external body force, recognizing that  and assuming that the body forces  and  do not depend on ,



### Discretization

Let



where  represents the interpolation functions over an element,  respectively represent nodal values of , and  is the number of nodes in an element. Then the discretized form of  in Eq. may be written as

,

where  is the number of elements in ,  is the number of integration points in the th element,  is the quadrature weight associated with the th integration point, and  is the Jacobian of the transformation from the spatial frame to the parametric space of the element. In the above expression,



and it is understood that ,  and  are evaluated at the parametric coordinates of the th integration point.

Similarly, the discretized form of  in Eqs. and may be written as

,

where



and  is a discrete increment in time. In a numerical implementation, it has been found that evaluating  from , where , yields more accurate solutions than evaluating it from the trace of  [[28](#_ENREF_28)].

For the various types of contributions to the external virtual work, a similar discretization produces

,

and

,

where

.

In this case,  represents the number of nodes on an element face. For a prescribed normal traction  as given in -,



where  is the skew-symmetric tensor whose dual vector is  and  is the third-order permutation pseudo-tensor. For a prescribed traction  as given in -,



For a prescribed normal fluid flux  as given in -,



## Weak Formulation for Biphasic-Solute Materials

The virtual work integral for this problem is given by

,

where  is the virtual velocity of the solid,  is the virtual effective fluid pressure, and  is the virtual molar energy of the solute.  represents the mixture domain in the spatial frame and  is an elemental mixture volume in . In the last integral of , note that

,

where  is the material time derivative of a scalar function  in the spatial frame, following the solid. Similarly, note that . Using the divergence theorem, the virtual work integral may be separated into internal and external contributions, , where



with  being evaluated on the domain’s boundary surface . In the first expression  represents the virtual solid rate of deformation.

To solve this nonlinear system using an iterative Newton scheme, the virtual work must be linearized at trial solutions, along increments in ,  and ,

,

where, for any function ,  represents the directional derivative of  along  [[1](#_ENREF_1)]. To operate the directional derivative on the integrand of , it is first necessary to convert the integrals from the spatial to the material domain [[1](#_ENREF_1)]:

,

where  represents the mixture domain in the material frame,  is an elemental mixture volume in , and



The second Piola-Kirchhoff stress tensor , and material flux vectors  and , are respectively related to ,  and  by the Piola transformations for tensors and vectors [[1](#_ENREF_1), [29](#_ENREF_29)]. Substituting into produces



where  and  are the material representations of the permeability and diffusivity tensors, related to  and  via the Piola transformation,



The linearization of  is rather involved and a summary of the resulting lengthy expressions is provided below. In consideration of the dearth of experimental data relating  and  to the complete state of solid matrix strain (such as ), this implementation assumes that the dependence of these functions on the strain is restricted to a dependence on the relative volume . Furthermore, it is assumed that the free solution diffusivity  is independent of the strain.

The linearization of  is described in Section 3.3.2. Following the linearization procedure, the resulting expressions may be discretized by nodally interpolating ,  and  over finite elements, producing a set of equations in matrix form, as described in Section 3.3.2.

The formulation presented in this study is implemented in FEBio by introducing an additional module dedicated to solute transport in deformable porous media. Classes are implemented to describe material functions for , ,  (and ),  and , which allow the formulation of any desired constitutive relation for these functions of  and , along with corresponding derivatives of these functions with respect to  and . The implementation accepts essential boundary conditions on ,  and , or natural boundary conditions on ,  and ; initial conditions may also be specified for  and . Analysis results for pressure and concentration may be displayed either as  and , or as  and  by inverting the relations of .

### Linearization of Internal Virtual Work

The virtual work integral  in may be linearized term by term along increments in ,  and  using the general form

.

For notational simplicity, the integral sign is omitted and the linearization of each term is presented in the form .

#### Linearization along

The linearization of the first term in  along  yields

,

where  is the spatial elasticity tensor of the mixture,

,

and  is the spatial elasticity tensor of the solid matrix,

.

The linearization of the second term is

,

where



with



representing the spatial tangents, with respect to the strain, of the effective permeability and solute diffusivity, respectively. These fourth-order tensors exhibit minor symmetries but not major symmetry, as described recently [[21](#_ENREF_21)]. Since  is given by substituting  into , the evaluation of  is rather involved and it can be shown that

,

where



and

.

The next term in  linearizes to

,

where

,

and  represents the time increment relative to the previous time point. The next term is given by

,

where



The last term is



#### Linearization along

The linearization of the various terms in  along  yields

,

,

.

#### Linearization along

The linearization of the first term in  along  yields

,

where



represents the spatial tangent of the stress with respect to the effective concentration. The next term is

,

where



and



is the spatial tangent of the effective hydraulic permeability with respect to the effective concentration.

The next term reduces to

.

The following term is

,

where



and



is the spatial tangent of the diffusivity with respect to the effective concentration.

The last term is



where

.

### Linearization of External Virtual Work

The linearization of  in depends on whether natural boundary conditions are prescribed as area densities or total net values over an area. Thus, in the case when  (net force),  (net volumetric flow rate), or  (net molar flow rate) are prescribed over the elemental area , there is no variation in  and it follows that . Alternatively, in the case when ,  or  are prescribed, the linearization may be performed by evaluating the integral in the parametric space of the boundary surface , with parametric coordinates . Accordingly, for a point  on , surface tangents (covariant basis vectors) are given by



and the outward unit normal is

.

The elemental area on  is . Consequently, the external virtual work integral may be rewritten as

.

The directional derivative of  may then be applied directly to its integrand, since the parametric space is invariant [[1](#_ENREF_1)].

If we restrict traction boundary conditions to the special case of normal tractions, then  where  is the prescribed normal traction component. Then it can be shown that the linearization of  along  produces

.

The linearizations along  and  reduce to zero,  and .

### Discretization

To discretize the virtual work relations, let



where  represents the interpolation functions over an element, , , , ,  and  respectively represent the nodal values of , , , ,  and ;  is the number of nodes in an element.

The discretized form of  in may be written as

,

where  is the number of elements in ,  is the number of integration points in the th element,  is the quadrature weight associated with the th integration point, and  is the Jacobian of the transformation from the current spatial configuration to the parametric space of the element. In the above expression,



and it is understood that , ,  and  are evaluated at the parametric coordinates of the th integration point. Since the parametric space is invariant, time derivatives are evaluated in a material frame. For example, the time derivative  appearing in becomes  when evaluated at the parametric coordinates  of the th integration point.

Similarly, the discretized form of  may be written as

,

where the terms in the first column are the discretized form of the linearization along :

,

,

,

where





,

.

The terms in the second column of the stiffness matrix in are the discretized form of the linearization along :

,

,

.

The terms in the third column of the stiffness matrix in are the discretized form of the linearization along :

,

,

,

where



,



The discretization of  in has the form

,

where . The summation is performed over all surface elements on which these boundary conditions are prescribed. The discretization of  has the form

,

where



In this expression,  is the antisymmetric tensor whose dual vector is  (such that  for any vector ).

## Weak Formulation for Multiphasic Materials

The virtual work integral for a mixture of intrinsically incompressible constituents combines the balance of momentum for the mixture, the balance of mass for the mixture, and the balance of mass for each of the solutes. In addition, for charged mixtures, the condition of may be enforced as a penalty constraint on each solute mass balance equation:



where  is the virtual velocity of the solid,  is the virtual effective fluid pressure, and  is the virtual molar energy of solute . Here,  represents the mixture domain in the spatial frame and  is an elemental volume in . Applying the divergence theorem,  may be split into internal and external contributions to the virtual work, , where



and

.

In these expressions, ,  is the boundary of , and $da$ is an elemental area on . In this finite element formulation, ,  and  are used as nodal variables, and essential boundary conditions may be prescribed on these variables. Natural boundary conditions are prescribed to the mixture traction, , normal fluid flux, , and normal solute flux, , where  is the outward unit normal to . To solve the system  for nodal values of ,  and , it is necessary to linearize these equations, as shown for example in Sections 3.3.1-3.3.2 for biphasic-solute materials. If the mixture is charged, it is also necessary to solve for the electric potential  by solving the algebraic relation of the electroneutrality condition in , which may be rewritten as

.

In the special case of a triphasic mixture, where solutes consist of two counter-ions (), this equation may be solved in closed form to produce

, 

Only the positive root is valid in the argument of the logarithm function.

### Chemical Reactions

The contribution to  due to chemical reactions is given by , where

. (3.122)

.

## Newton-Raphson Method

The Newton-Raphson method (also known as “Newton’s method”, “Full Newton method” or “the Newton method”) is the basis for solving the nonlinear finite element equations. This section will describe the *Full Newton method* and the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method [[30](#_ENREF_30)]. The latter variation is actually a *quasi-Newton method*. It is important since it provides several advantages over the full Newton method and it is this method that is implemented in FEBio [[30](#_ENREF_30)].

### Full Newton Method

The Newton-Raphson equation can be written in terms of the discretized equilibrium equations that were derived in the previous section as follows:

.

Since the virtual velocities are arbitrary, a discretized Newton-Raphson scheme can be formulated as follows:

.

This is the basis of the Newton-Raphson method. For each iteration *k*, both the stiffness matrix and the residual vector are re-evaluated and a displacement increment **u** is calculated by pre-multiplying both sides of the above equation by . This procedure is repeated until some convergence criteria are satisfied.

The formation of the stiffness matrix and, especially, calculation of its inverse, are computationally expensive. Quasi-Newton methods do not require the reevaluation of the stiffness matrix for every iteration. Instead, a quick update is calculated. One particular method that has been quite successful in the field of computational solid mechanics is the BFGS method, which is described in the next section.

### BFGS Method

The BFGS method updates the stiffness matrix (or rather its inverse) to provide an approximation to the exact matrix. A displacement increment is defined as

,

and an increment in the residual is defined as

.

The updated matrix should satisfy the quasi-Newton equation:

.

In order to calculate this update, as displacement increment is first calculated:

.

This displacement vector defines a “direction” for the actual displacement increment. A line search (see next section) can now be applied to determine the optimal displacement increment:

,

where *s* is determined from the line search. With the updated position calculated, can be evaluated. Also, using equations and , and  can be evaluted. The stiffness update can now be expressed as

,

where the matrix **A** is an  matrix of the simple form:

.

The vectors **v** and **w** are given by

,

.

The vector is equal to and has already been calculated.

To avoid numerically dangerous updates, the condition number *c* of the updating matrix **A** is calculated:

.

The update is not performed when this number exceeds a preset tolerance.

Considering the actual computations involved, it should be noted that using the matrix updates defined above, the calculation of the search direction in can be rewritten as,

.

Hence, the search direction can be computed without explicitly calculating the updated matrices or performing any additional costly matrix factorizations as required in the full Newton-Raphson method.

### Line Search Method

A powerful technique often used to improve the convergence rate of Newton based methods is the *line search method*. In this method, the direction of the displacement vector **u** is considered as optimal, but the magnitude is controlled by a parameter *s*:

.

The value of *s* is usually chosen so that the total potential energy at the end of the iteration is minimized in the direction of **u**. This is equivalent to the requirement that the residual force at the end of the iteration is orthogonal to **u**:

.

However, in practice it is sufficient to obtain a value of *s* such that,

,

where typically a value of is used. Under normal conditions the value  automatically satisfies equation and therefore few extra operations are involved. However, when this is not the case, a more suitable value for *s* needs to be obtained. For this reason it is convenient to approximate as a quadratic in *s*:

,

which yields a value for *s* as

.

If , the square root is positive and a first improved value for *s* is obtained:

.

If  the *s* can be obtained by using the value that minimizes the quadratic function, that is, . This procedure is now repeated with  replaced by  until equation is satisfied.

# Element Library

FEBio provides several element types for finite element discretization. This chapter describes these elements in more detail.

## Solid Elements

The 3D solid elements available in FEBio are *isoparametric elements*. All of the solid elements are formulated in a global Cartesian coordinate system. For all these elements, a local coordinate system (so-called *isoparametric coordinates*) is defined as well. The global position vector **x** can be written as a function of the isoparametric coordinates in the following sense:

.

Here, *n* is the number of nodes, *r*, *s* and *t* are the isoparametric coordinates,  are the element shape functions and  are the spatial coordinates of the element nodes. The same parametric interpolation is used for the interpolation of other scalar and vector quantities.

All elements in FEBio are integrated numerically. This implies that integrals over the volume of the element *ve* are approximated by a sum:

.

Here,  is the biunit cube, *m* is the number of integration points, are the location of the integration points in isoparametric coordinates, *J* is the Jacobian of the transformation , and is a weight associated with the integration point. The integration is performed over the element’s volume in the natural coordinate system.

Most fully integrated solid elements are unsuitable for the analysis of (nearly-) incompressible material behavior. To deal with this type of deformation, a three-field element implementation is available in FEBio [[31](#_ENREF_31)].

### Hexahedral Elements

FEBio implements an 8-node trilinear hexahedral element. This element is also known as a *brick* element. The shape functions for these elements are defined in function of the isoparametric coordinates *r*, *s* and *t,* and are given below.



The following integration rule is implemented for this element type.

**8-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| -0.577350269 | -0.577350269 | -0.577350269 | 1 |
| 0.577350269 | -0.577350269 | -0.577350269 | 1 |
| 0.577350269 | 0.577350269 | -0.577350269 | 1 |
| -0.577350269 | 0.577350269 | -0.577350269 | 1 |
| -0.577350269 | -0.577350269 | 0.577350269 | 1 |
| 0.577350269 | -0.577350269 | 0.577350269 | 1 |
| 0.577350269 | 0.577350269 | 0.577350269 | 1 |
| -0.577350269 | 0.577350269 | 0.577350269 | 1 |

### Pentahedral Elements

Pentahedral elements (also knows as “wedge” elements) consist of six nodes and five faces. Their shape functions are defined in function of the isoparametric coordinates *r*, *s* and *t* and are given as follows.



The following integration rule is implemented for this element type.

**6-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.166666667 | 0.166666667 | -0.577350269 | 0.166666667 |
| 0.666666667 | 0.166666667 | -0.577350269 | 0.166666667 |
| 0.166666667 | 0.666666667 | -0.577350269 | 0.166666667 |
| 0.166666667 | 0.166666667 | 0.577350269 | 0.166666667 |
| 0.666666667 | 0.166666667 | 0.577350269 | 0.166666667 |
| 0.166666667 | 0.666666667 | 0.577350269 | 0.166666667 |

### Tetrahedral Elements

Linear 4-node tetrahedral elements are also available in FEBio. Their shape functions are defined in function of the isoparametric coordinates *r*, *s* and *t*.



The following integration rules are implemented for this element type.

**1-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.25 | 0.25 | 0.25 | 0.166666667 |

**4-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.13819660 | 0.13819660 | 0.13819660 | 0.041666667 |
| 0.58541020 | 0.13819660 | 0.13819660 | 0.041666667 |
| 0.13819660 | 0.58541020 | 0.13819660 | 0.041666667 |
| 0.13819660 | 0.13819660 | 0.58541020 | 0.041666667 |



Figure 4‑1. Different solid element types that are available in FEBio.

### Quadratic Tetrahedral Elements

FEBio implements a 10-node quadratic tetrahedral element. It has four corner nodes and six nodes located at the midpoint of the edges. The shape functions in terms area coordinates are given below. The area coordinates relate to the isoparametric coordinates as follows.



The shape functions follow.



The following integration rules are implemented for this element type.

**4-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.58541020 | 0.13819660 | 0.13819660 | 0.041666667 |
| 0.13819660 | 0.58541020 | 0.13819660 | 0.041666667 |
| 0.13819660 | 0.13819660 | 0.58541020 | 0.041666667 |
| 0.13819660 | 0.13819660 | 0.13819660 | 0.041666667 |

**8-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.01583591 | 0.328054697 | 0.328054697 | 0.023087995 |
| 0.328054697 | 0.01583591 | 0.328054697 | 0.023087995 |
| 0.328054697 | 0.328054697 | 0.01583591 | 0.023087995 |
| 0.328054697 | 0.328054697 | 0.328054697 | 0.023087995 |
| 0.679143178 | 0.106952274 | 0.106952274 | 0.018578672 |
| 0.106952274 | 0.679143178 | 0.106952274 | 0.018578672 |
| 0.106952274 | 0.106952274 | 0.679143178 | 0.018578672 |
| 0.106952274 | 0.106952274 | 0.106952274 | 0.018578672 |

**11-point Gauss-Lobatto rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0 | 0 | 0 | 0.002777778 |
| 1 | 0 | 0 | 0.002777778 |
| 0 | 1 | 0 | 0.002777778 |
| 0 | 0 | 1 | 0.002777778 |
| 0.5 | 0 | 0 | 0.011111111 |
| 0.5 | 0.5 | 0 | 0.011111111 |
| 0 | 0.5 | 0 | 0.011111111 |
| 0 | 0 | 0.5 | 0.011111111 |
| 0.5 | 0 | 0.5 | 0.011111111 |
| 0 | 0.5 | 0.5 | 0.011111111 |
| 0.25 | 0.25 | 0.25 | 0.088888889 |

FEBio also implements a 15-node quadratic tetrahedral element (see Figure 4‑2).

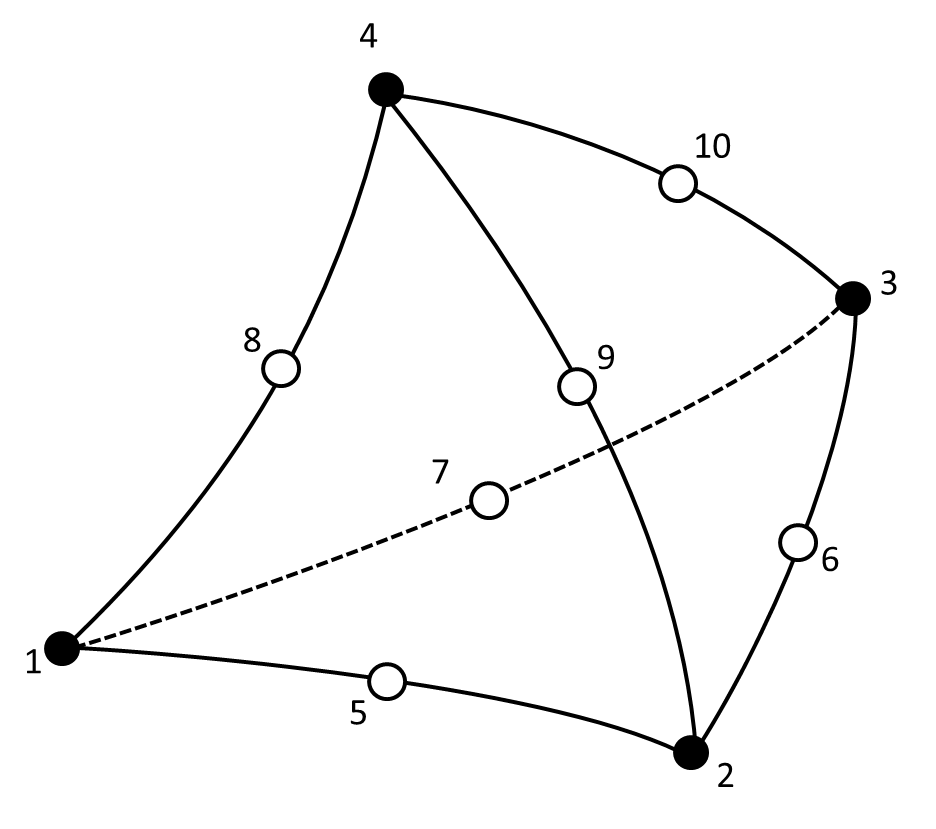


Figure 4‑2 Quadratic tetrahedral elements available in FEBio. Left, a 10-node quadratic tet. Right, a 15-node quadratic tet.

The following integration rules are implemented for this element type.

**8-point Gauss rule[[1]](#footnote-1)**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.0158359099 | 0.3280546970 | 0.3280546970 | 0.138527967 |
| 0.3280546970 | 0.0158359099 | 0.3280546970 | 0.138527967 |
| 0.3280546970 | 0.3280546970 | 0.0158359099 | 0.138527967 |
| 0.3280546970 | 0.3280546970 | 0.3280546970 | 0.138527967 |
| 0.6791431780 | 0.1069522740 | 0.1069522740 | 0.111472033 |
| 0.1069522740 | 0.6791431780 | 0.1069522740 | 0.111472033 |
| 0.1069522740 | 0.1069522740 | 0.6791431780 | 0.111472033 |
| 0.1069522740 | 0.1069522740 | 0.1069522740 | 0.111472033 |

**11-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.25 | 0.25 | 0.25 | -0.01315555556 |
| 0.071428571428571 | 0.071428571428571 | 0.071428571428571 | 0.007622222222 |
| 0.785714285714286 | 0.071428571428571 | 0.071428571428571 | 0.007622222222 |
| 0.071428571428571 | 0.785714285714286 | 0.071428571428571 | 0.007622222222 |
| 0.071428571428571 | 0.071428571428571 | 0.785714285714286 | 0.007622222222 |
| 0.399403576166799 | 0.100596423833201 | 0.100596423833201 | 0.024888888889 |
| 0.100596423833201 | 0.399403576166799 | 0.100596423833201 | 0.024888888889 |
| 0.100596423833201 | 0.100596423833201 | 0.399403576166799 | 0.024888888889 |
| 0.399403576166799 | 0.399403576166799 | 0.100596423833201 | 0.024888888889 |
| 0.399403576166799 | 0.100596423833201 | 0.399403576166799 | 0.024888888889 |
| 0.100596423833201 | 0.399403576166799 | 0.399403576166799 | 0.024888888889 |

**15-point Gauss rule**

|  |  |  |  |
| --- | --- | --- | --- |
| **r** | **s** | **t** | **w** |
| 0.25 | 0.25 | 0.25 | 0.030283678097089 |
| 0.333333333333333 | 0.333333333333333 | 0.333333333333333 | 0.006026785714286 |
| 0.000000000000000 | 0.333333333333333 | 0.333333333333333 | 0.006026785714286 |
| 0.333333333333333 | 0.000000000000000 | 0.333333333333333 | 0.006026785714286 |
| 0.333333333333333 | 0.333333333333333 | 0.000000000000000 | 0.006026785714286 |
| 0.090909090909091 | 0.090909090909091 | 0.090909090909091 | 0.011645249086029 |
| 0.727272727272727 | 0.090909090909091 | 0.090909090909091 | 0.011645249086029 |
| 0.090909090909091 | 0.727272727272727 | 0.090909090909091 | 0.011645249086029 |
| 0.090909090909091 | 0.090909090909091 | 0.727272727272727 | 0.011645249086029 |
| 0.433449846426336 | 0.066550153573664 | 0.066550153573664 | 0.010949141561386 |
| 0.066550153573664 | 0.433449846426336 | 0.066550153573664 | 0.010949141561386 |
| 0.066550153573664 | 0.066550153573664 | 0.433449846426336 | 0.010949141561386 |
| 0.066550153573664 | 0.433449846426336 | 0.433449846426336 | 0.010949141561386 |
| 0.433449846426336 | 0.066550153573664 | 0.433449846426336 | 0.010949141561386 |
| 0.433449846426336 | 0.433449846426336 | 0.066550153573664 | 0.010949141561386 |

## Shell Elements

Historically, shells have been formulated using two different approaches [[32](#_ENREF_32)]. The difference between these approaches lies in the way the rotational degrees of freedom are defined. In the first approach, the rotational degrees of freedom are defined as angles. In addition, the plane stress condition needs to be enforced to take thickness variations into account. This approach is very useful for infinitesimal strains, but becomes very difficult to pursue in finite deformation due to the fact that finite rotations do not commute. Another disadvantage of this approach is that it requires a modification to the material formulation to enforce the plane stress condition. For complex materials this modification is very difficult or even impossible to obtain.

The alternative approach is to use an *extensible director* to describe the rotational degrees of freedom. With this approach it is not necessary to enforce the plane-stress condition and the full 3D constitutive relations can be employed. This approach is used in FEBio. A disadvantage of this approach is that it becomes difficult to enforce the unit length of the director throughout the entire element.

The shell formulation implemented in FEBio is still a work in progress. The goal is to implement an extensible director formulation with strain enhancements to deal with the well-known locking effect in incompressible and bending problems [[33](#_ENREF_33)]. With the current state of the implementation, it is advised to use a fine mesh in such problems.

### Shell formulation

In FEBio an extensible director formulation is implemented [[33](#_ENREF_33)]. Six degrees of freedom are assigned to each shell node: three displacement degrees of freedom and three director degrees of freedom. The position of any point in the shell can be written as:



It is assumed that Latin indices range from 1 to 3 and that Greek indices range from 1 to 2. The vector **D** is called the *director* and it is assumed that . (Note that this does not necessarily imply that  throughout the entire shell.) The function is the *thickness function* and evaluates the initial thickness of the shell, which at node *a* is given by .

Similarly, the displacement is given by



The current configuration is then determined by



To take thickness variations into account, it is not required that is of unit length.

It is assumed that the virtual displacements have a similar interpolation than the actual displacements:

.

The gradient of **u** is given by

.

where we have defined . And similarly for the gradient of the virtual displacement,

.

The internal virtual work is now given by



The shell geometry suggests an integration of the following type:

.

where is the Jacobian of the transformation. In FEBio a 3-point Gaussian quadrature rule is used for the through-the-thickness integration.

FEBio currently supports four node quadrilateral and three-node triangular shell elements.

### Quadrilateral shells

For quadrilateral shells, the shape functions are given by



### Triangular shells

For triangular shell elements, the shape functions are given by



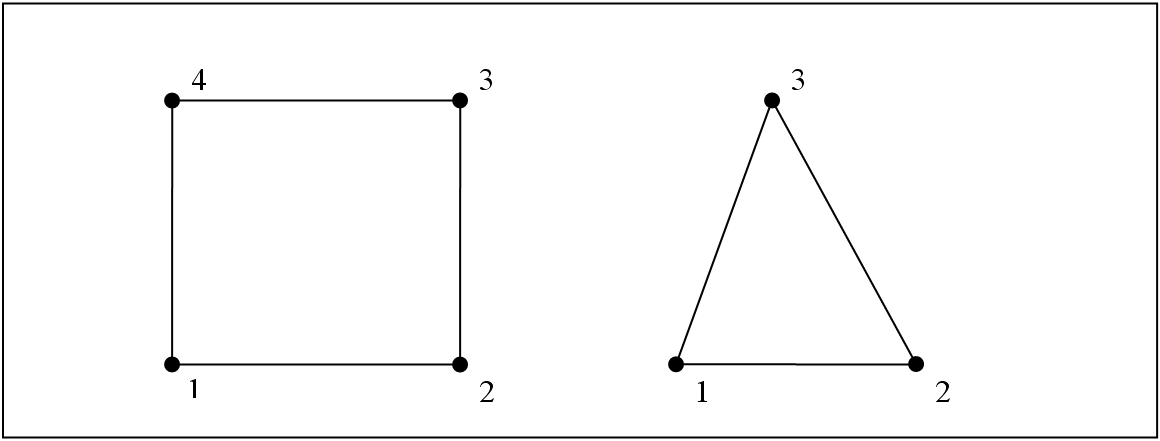


Figure 4‑3. Different shell elements available in FEBio

# Constitutive Models

This chapter describes the theoretical background behind the constitutive models that are available in FEBio. Most materials are derived from a hyperelastic strain-energy function. Please consult section 2.4 for more background information on this class of materials.

## Linear Elasticity

In the theory of linear elasticity the Cauchy stress tensor is a linear function of the small strain tensor :

.

Here, is the fourth-order elasticity tensor that contains the material properties. In the most general case this tensor has 21 independent parameters. However, in the presence of material symmetry the number of independent parameters is greatly reduced. For example, in the case of isotropic linear elasticity only two independent parameters remain. In this case, the elasticity tensor is given by , or equivalently,

.

The material coefficients  and are known as the Lamé parameters. Using this equation, the stress-strain relationship can be written as

.

If the stress and strain are represented inVoigt notation, the constitutive equation can be rewritten in matrix form as

.

The shear strain measures  are called the *engineering strains*.

The following table relates the Lamé parameters to the more familiar Young’s modulus *E* and Poisson’s ratio or to the bulk modulus *K* and shear modulus *G*.

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |

The theoretical range of the Young’s modulus and Poisson’s ratio for an isotropic material have the ranges

,

.

Materials with Poisson’s ratio (close to) 0.5 are known as (nearly-) incompressible materials. For these materials, the bulk modulus approaches infinity. Most materials have a positive Poisson’s ratio. However there do exist some materials with a negative ratio. These materials are known as *auxetic* materials and they have the remarkable property that they expand under tension.

The linear stress-strain relationship can also be derived from a strain-energy function such as in the case of hyperelastic materials. In this case the linear strain-energy is given by

.

The stress is then similarly derived from . In the case of isotropic elasticity, can be simplified:

.

The Cauchy stress is now given in tensor form by

.

## Compressible Materials

### Isotropic Elasticity

The linear elastic material model as described in section 5.1 is only valid for small strains and small rotations. A first modification to this model to the range of nonlinear deformations is given by the St. Venant-Kirchhoff model [[1](#_ENREF_1)], which in FEBio is referred to as *isotropic elasticity*. This model is objective for large strains and rotations. For the isotropic case it can be derived from the following hyperelastic strain-energy function:

.

The second Piola-Kirchhoff stress can be derived from this:

.

Note that these equations are similar to the corresponding equations in the linear elastic case, except that the small strain tensor is replaced by the Green-Lagrange elasticity tensor **E**. The material elasticity tensor is then given by,

.

It is important to note that although this model is objective, it should only be used for small strains. For large strains, the response can be somewhat strange if not completely unrealistic. For example, it can be shown that under uni-axial tension the stress becomes infinite and the volume tends to zero for finite strains. Therefore, for large strains it is highly recommended to avoid this material and instead use one of the other non-linear material models described below. The Cauchy stress is



where  , whereas the spatial elasticity tensor is



### Orthotropic Elasticity

An extension of the St. Venant-Kirchhoff model [[1](#_ENREF_1)] to orthotropic symmetry is provided in FEBio, referred to as *orthotropic elasticity*. This model is objective for large strains and rotations. It can be derived from the following hyperelastic strain-energy function:

,

where  is the structural tensor corresponding to one of the three mutually orthogonal planes of symmetry whose unit outward normal is  (). The material constants are the three shear moduli  and six moduli , where . They may be related to the Young’s moduli , shear moduli  and Poisson’s ratios  via



The second Piola-Kirchhoff stress can be derived from this strain energy density function:



Note that these equations are similar to the corresponding equations in the linear orthotropic elastic case, except that the small strain tensor is replaced by the Green-Lagrange elasticity tensor . The material elasticity tensor is then given by,

.

It is important to note that although this model is objective, it should only be used for small strains. For large strains, the response can be somewhat strange if not completely unrealistic. For example, it can be shown that under uni-axial tension the stress becomes infinite and the volume tends to zero for finite strains. Therefore, for large strains it is highly recommended to avoid this material and instead use one of the other non-linear material models described below. The Cauchy stress is



where  and the spatial elasticity tensor is



### Neo-Hookean Hyperelasticity

This is a compressible neo-Hookean material. It is derived from the following hyperelastic strain energy function [[1](#_ENREF_1)]:

.

The parameters  and  are the Lamé parameters from linear elasticity. This model reduces to the isotropic linear elastic model for small strains and rotations.

The Cauchy stress is given by,

,

and the spatial elasticity tensor is given by,

.

The neo-Hookean material is an extension of Hooke’s law for the case of large deformations. It is useable for certain plastics and rubber-like substances. A generalization of this model is the Mooney-Rivlin material, which is often used to describe the elastic response of biological tissue.

In FEBio this constitutive model uses a standard displacement-based element formulation and a "coupled" strain energy, so care must be taken when modeling materials with nearly-incompressible material behavior to avoid element locking.

### Ogden Unconstrained

The Ogden unconstrained material is defined using the following hyperelastic strain energy function:

.

Here,  are the principal stretches and , and  are material parameters.

The Cauchy stress tensor for this material may be obtained using the general formula for isotropic elasticity in principal directions given in , with

.

Similarly, the spatial elasticity tensor is given by



where  and  are the eigenvectors of . In the limit when eigenvalues coincide,

.

In the reference configuration, the elasticity tensor reduces to

,

which has the form of Hooke’s law for infinitesimal isotropic elasticity (see Section 5.1), with equivalent Lamé coefficients  and .

### Holmes-Mow

The coupled hyperelastic strain-energy function for this material is given by [[34](#_ENREF_34)],

,

where and are the first and second invariants of the right Cauchy-Green tensor and *J* the jacobian of the deformation. Furthermore,



and and  are the Lamé parameters. The corresponding Cauchy stress tensor is

,

and the spatial elasticity tensor is

.

### Conewise Linear Elasticity

Curnier et al. [[27](#_ENREF_27)] formulated a model for describing bimodular elastic solids exhibiting orthotropic material symmetry. This can be derived from the following hyperelastic strain-energy function:

,

where  is the structural tensor corresponding to one of the three mutually orthogonal planes of symmetry whose unit outward normal is  (). The bimodular response is described by



The material constants are the three shear moduli , three tensile moduli , three compressive moduli , and three moduli  (), where . The second Piola-Kirchhoff stress can be derived from this strain energy density function:



The material elasticity tensor is then given by,

.

It is important to note that although this model is objective, it should only be used for small strains. For large strains, the response may be unrealistic. The Cauchy stress is



where  and . The spatial elasticity tensor is



In the special case of cubic symmetry, the number of material constants reduces to four,



### Donnan Equilibrium Swelling

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. Since osmotic swelling must be resisted by a solid material, this material is not stable on its own. It must be combined with an elastic material that resists the swelling.

The Cauchy stress for this material is the stress from the Donnan equilibrium response [[35](#_ENREF_35)]:

,

where  is the osmotic pressure, given by

,

and  is the fixed charge density in the current configuration, related to the reference configuration via,

,

where  is the relative volume, is the universal gas constant and  is the absolute temperature.

Note that  may be negative or positive. The gel porosity is unitless and must be in the range . The corresponding spatial elasticity tensor is [[36](#_ENREF_36)]



### Perfect Osmometer Equilibrium Osmotic Pressure

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.

The Cauchy stress for this material is the stress from the perfect osmometer equilibrium response [[14](#_ENREF_14)]:

,

where  is the osmotic pressure, given by

.

 is the interstitial fluid in the current configuration, related to the reference configuration via,

,

where is the universal gas constant and  is the absolute temperature.

Though this material is porous, this is not a full-fledged poroelastic material. The behavior described by this material is strictly valid only after the transient response of interstitial fluid and solute fluxes as subsided. The corresponding spatial elasticity tensor is

.

## Nearly-Incompressible Materials

### Mooney-Rivlin Hyperelasticity

This material model is a hyperelastic Mooney-Rivlin type with uncoupled deviatoric and volumetric behavior. The uncoupled strain energy W is given by:

.

Here,  and  are the Mooney-Rivlin material coefficients,  and  are the invariants of the deviatoric part of the right Cauchy-Green deformation tensor, , where , ***F*** is the deformation gradient and  is the Jacobian of the deformation. When , this model reduces to an uncoupled version of the incompressible neo-Hookean constitutive model.

The Cauchy stress is given by

.

The spatial elasticity tensor is given by

,

where,



This material model uses a three-field element formulation, interpolating displacements as linear field variables and pressure and volume ratio as piecewise constant in each element [[31](#_ENREF_31)].

### Ogden Hyperelastic

The Ogden material is defined using the following hyperelastic strain energy function:

.

Here,  are the deviatoric principal stretches and  and  are material parameters. The term is the volumetric component and *J* is the determinant of the deformation gradient.

Note that the neo-Hookean and Mooney-Rivlin models can also be obtained from the general Ogden strain energy function using special choices for  and .

### Veronda-Westmann Hyperelasticity

This model is similar to the Mooney-Rivlin model in that it also uses an uncoupled strain energy. However, in this case the strain energy is given by an exponential form:

.

The dilatational term *U* is identical to the Mooney-Rivlin model.

The Cauchy stress  is found from

,

where

.

The strain energy derivatives are given by

,

.

This material model was the result from the research of the elastic response of skin tissue [[37](#_ENREF_37)].

### Arruda-Boyce Hyperelasticity

Arruda and Boyce proposed a model for the deformation of rubber materials [[38](#_ENREF_38)]. Their main motivation was to develop a model that accurately captures the behavior of rubbers in different loading scenarios and that can be described with a limited number of physically motivated parameters. Their model is based on the Langevin chain statistics, which models a rubber chain segment between chemical crosslinks as a number  of rigid links of equal length . The parameter  is related to the locking stretch , the stretch at which the chains reach their full extended state, .

Their proposed strain-energy is a truncated Taylor series of the inverse Langevin function. A formulation that retains the first five terms of this function takes on the following form:

,

where  is a shear-modulus like parameter and the coefficients  are



The Cauchy stress is given by

,

where,

.

### Transversely Isotropic Hyperelastic

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 [[5](#_ENREF_5), [39](#_ENREF_39), [40](#_ENREF_40)]. 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 strain energy function can be written as follows:

.

Here and  are the first and second invariants of the deviatoric version of the right Cauchy Green deformation tensor and  is the deviatoric part of the stretch along the fiber direction (, where  is the initial fiber direction). The function  represents the material response of the isotropic ground substance matrix, while represents the contribution from the fiber family. The strain energy of the fiber family is as follows:



Here,  is the stretch at which the fibers are straightened,  scales the exponential stresses,  is the rate of uncrimping of the fibers, and  is the modulus of the straightened fibers.  is determined from the requirement that the stress is continuous at .

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 [[31](#_ENREF_31)].

### Ellipsoidal Fiber Distribution

This constitutive model describes a material that is composed of an ellipsoidal continuous fiber distribution in an uncoupled formulation. The deviatoric part of the stress is given by [[35](#_ENREF_35), [41](#_ENREF_41), [42](#_ENREF_42)],

,

and the corresponding elasticity tensor is

.

 is the square of the fiber stretch ,  is the unit vector along the fiber direction (in the reference configuration), which in spherical angles is directed along ,  and  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:

,

whereas the fiber elasticity tensor is

,

where in this material

.

The materials parameters  and  are determined from:



Since fibers can only sustain tension, this material is not stable on its own. It must be combined with a material that acts as the ground matrix. The total stress is then given by the sum of the fiber stress and the ground matrix stress:

.

### Fiber with Exponential Power law

This material model describes a constitutive model for fibers, where a single fiber family follows an exponential power law strain energy function. The deviatoric part of the Cauchy stress is given by:

,

and the corresponding spatial elasticity tensor is



where  is the square of the fiber stretch,  is the fiber orientation in the reference configuration,



and  and  is the unit step function that enforces the tension-only contribution. The fiber strain energy density is given by

,

where , and .

Note: in the limit when , this expression produces a power law,

.

Note: when , the fiber modulus is zero at the strain origin (). Therefore, use when a smooth transition in the stress is desired from compression to tension.

### Fung Orthotropic

The hyperelastic strain energy function for a Fung Orthotropic material is given by [[43](#_ENREF_43), [44](#_ENREF_44)]

,

where

.

Here,  and , where  are orthonormal vectors that define the initial direction of material axes. The orthotropic Lamé coefficients should be chosen such that the stiffness matrix,



is positive definite.

### Tension-Compression Nonlinear Orthotropic

This material model is based on the following uncoupled hyperelastic strain energy function [[45](#_ENREF_45)]:

.

The isotropic strain energy and the dilatational energy *U* are the same as for the Mooney-Rivlin material. The tension-compression term is defined as follows:



The  parameters are the deviatoric fiber stretches of the local material fibers,

.

The local material fibers are defined (in the reference frame) as an orthonormal set of vectors . The corresponding deviatoric part of the Cauchy stress is



and the spatial elasticity tensor is



where .

## Viscoelasticity

For a viscoelastic material the second Piola Kirchhoff stress can be written as follows [[39](#_ENREF_39)]:

,

where is the elastic stress and *G*(*t*) is the relaxation function. Here we consider the special case where the relaxation function is given by

.

With this function chosen for the relaxation function, we can write the total stress as

.

Introducing the internal variables,

,

we can rewrite as follows,

.

In FEBio, , so  is the long-term elastic response of the material.

The question now remains how to evaluate the internal variables. From equation it appears that we have to integrate over the entire time domain. However, we can find a recurrence relationship that will allow us to evaluate the internal variables at a time given the values at time *t*.



The last term can now be simplified using the midpoint rule to approximate the derivate. In that case we find the recurrence relation:

.

The following procedure can now be applied to calculate the new stress. Given  and  corresponding to time *t*, find  and  corresponding to time :

1. calculate elastic stress: 
2. evaluate internal variables: 
3. find the total stress: 

## Reactive Viscoelasticity

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 [[46](#_ENREF_46)]. Strong bonds produce the equilibrium elastic response, whereas weak bonds produce the transient viscous response. Strong bonds are in a stress-free state when in their reference configuration . Their deformation gradient is defined as usual, . When weak bonds break in response to loading at some time , they reform instantaneously in a stress-free configuration  that coincides with the current configuration at time , thus, . Therefore, a reaction transforms intact loaded bonds into reformed unloaded bonds. Weak bonds that reform at time  may be called generation bonds. The deformation gradient of generation weak bonds relative to their reference configuration  is denoted by , which may be evaluated from the chain rule,



The strain energy density  in a reactive viscoelastic material is given by



where  is the strain energy density of strong bonds and  is the strain energy density of weak bonds, when they all belong to the same generation. In this expression,  is the mass fraction of generation weak bonds, which evolves over time as described below. The summation is taken over all generations  that were created prior to the current time . The Cauchy stress  in a reactive viscoelastic material is similarly given by



where  is the stress in the strong bonds and  is the stress in the weak bonds. These stresses are related to the respective strain energy densities of strong and weak bonds according to



The mass fractions  are obtained by solving the equation of mass balance for reactive constrained mixtures,



where the mass fraction supply  must be specified as a constitutive function of the deformation gradient  and the mass fractions  from all generations. Since mass must be conserved over all generations, it follows that



Any number of valid solutions may exist for , based on constitutive assumptions for . For example, for generation bonds reforming in an unloaded state during the time interval , and subsequently breaking in response to loading at , Type I bond kinetics provides a solution of the form



where



and  is a reduced relaxation function which may assume any number of valid forms. (A reduced relaxation function  satisfies  and , and decreases monotonically with .) In particular,  may depend on the strain at time  relative to the reference configuration of the generation. In the recursive expression of , the earliest generation , which is initially at rest, produces  for  and  for ; this latter expression seeds the recursion for subsequent generations. Therefore, providing a functional form for  suffices to produce the solution for all bond generations .

For Type II bond kinetics, the solution for the mass fractions is given by



For this type of bond kinetics, the reduced relaxation function  cannot depend on the magnitude of the strain, because strain-dependence might violate the constraint .

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.

The finite element implementation of reactive viscoelasticity stores the value of  every time that a bond-breaking deformation is detected; this value can be used to evaluate  using . It also stores , where  is the time step immediately following , which is then used for evaluating  for subsequent time steps  when using Type I bond kinetics, using the expressions of and . These measures are then used to evaluate the stress from , with the summation taken over the time steps that correspond to bond-reforming generations.

## Hydraulic Permeability

Hydraulic permeability is a material function needed for biphasic and biphasic-solute materials.

### Constant Isotropic Permeability

When the permeability is isotropic,

.

For this material model,  is constant. Generally, this assumption is only reasonable when strains are small.

### Holmes-Mow

This isotropic material is similar to the constant isotropic permeability material described above, except that it uses a strain-dependent permeability tensor [[34](#_ENREF_34)]:

,

where,

.

### Referentially Isotropic Permeability

This material uses a strain-dependent permeability tensor that accommodates strain-induced anisotropy [[21](#_ENREF_21)]:

,

Note that the permeability in the reference state () is isotropic and given by .

### Referentially Orthotropic Permeability

This material uses a strain-dependent permeability tensor that is orthotropic in the reference configuration, and accommodates strain-induced anisotropy [[21](#_ENREF_21)]:

,

where,



 are second order tensors representing the spatial structural tensors describing the orthogonal planes of symmetry, given by

,

where  are orthonormal vectors normal to the planes of symmetry. Note that the permeability in the reference state () is given by .

### Referentially Transversely Isotropic Permeability

This material uses a strain-dependent permeability tensor that is transversely isotropic in the reference configuration, and accommodates strain-induced anisotropy [[21](#_ENREF_21)]:



 is a second order tensor representing the spatial structural tensor describing the axial direction, given by

,

where  is a unit vector along the axial direction. Note that the permeability in the reference state () is given by .

## Solute Diffusivity

Diffusivity materials provide a constitutive relation for the solute diffusivity in a biphasic-solute material. In general, the diffusivity tensor  may be a function of strain and solute concentration.

### Constant Isotropic Diffusivity

When the permeability is isotropic,

.

For this material model,  is constant. This assumption is only true when strains are small. Note that the user must specify , where  is the solute diffusivity in free solution, since a solute cannot diffuse through the biphasic-solute mixture faster than in free solution.

### Constant Orthotropic Diffusivity

When the permeability is orthotropic,

,

where  are orthonormal vectors normal to the planes of symmetry. For this material model, the  are constant. Therefore this model should be used only when strains are small. Note that the user must specify , where  is the solute diffusivity in free solution, since a solute cannot diffuse through the biphasic-solute mixture faster than in free solution.

### Referentially Isotropic Diffusivity

This material uses a strain-dependent diffusivity tensor that is isotropic in the reference configuration and accommodates strain-induced anisotropy:

,

where is the jacobian of the deformation, i.e.  where is the deformation gradient, and  is the left Cauchy-Green tensor. Note that the diffusivity in the reference state () is isotropic and given by .

### Referentially Orthotropic Diffusivity

This material uses a strain-dependent diffusivity tensor that is orthotropic in the reference configuration and accommodates strain-induced anisotropy:

,

where,



 is the Jacobian of the deformation, i.e.  where **** is the deformation gradient.  are second order tensor representing the spatial structural tensors describing the orthogonal planes of symmetry, given by

,

where  are orthonormal vectors normal to the planes of symmetry. Note that the permeability in the reference state () is given by .

## Solute Solubility

Solubility constitutive equations provide a relation for  as a function of solid matrix strain and effective solute concentrations.

### Constant Solubility

For this material model,  is constant.

## Osmotic Coefficient

Osmotic coefficient constitutive equations provide a relation for  as a function of solid matrix strain and effective solute concentrations.

### Constant Osmotic Coefficient

For this material model,  is constant.

## Active Contraction Model

A time varying “elastance” active contraction model [[47](#_ENREF_47)] was added to the transversely isotropic materials. When active contraction is activated, the total Cauchy stress is defined as the sum of the active stress tensor  and the passive stress tensor :

,

where ***a*** is the deformed fiber vector (unit length), defined as . The time varying elastance model is a modification of the standard Hill equation that scales the standard equation by an activation curve . The active fiber stress  is defined as:

,

where *Tmax* = 135.7 KPa is the isometric tension under maximal activation at the peak intracellular calcium concentration of *Ca0* = 4.35 μM. The length dependent calcium sensitivity is governed by the following equation:

,

where (*Ca0*)*max* = 4.35 μM is the maximum peak intracellular calcium concentration, *B = 4.75* μm-1 governs the shape of the peak isometric tension-sarcomere length relation, *l0* = 1.58 μm is the sarcomere length at which no active tension develops, and *l* is the sarcomere length which is the product of the fiber stretch *λ* and the sarcomere unloaded length *lr = 2.04* μm.

## Prescribed Active Contraction

Prescribed active contraction models allow the user to directly specify the time history of the active contractile stress.

### Uniaxial Active Contraction

For this model, the active stress is acting along a prescribed direction given by the unit vector in the reference configuIation. The 2nd Piola-Kirchhoff stress is



and the Cauchy stress is



where  is the prescribed contractile stress and . Since  is not a function of deformation, the material and spatial tangents are both zero.

### Transversely Isotropic Active Contraction

In this case, the active stress is isotropic in a plane transverse to the direction ,



and the corresponding Cauchy stress is



where  is the left Cauchy-Green tensor. The material and spatial tangents are zero.

### Isotropic Active Contraction

An isotropic active contractile stress is given by



and the corresponding Cauchy stress is



The material and spatial tangents are zero.

## Chemical Reaction Production Rate

Production rate constitutive equations provide a relation for  as a function of solid matrix strain, solute concentrations, and the concentrations of solid-bound molecular species.

### Mass Action Forward

According to the law of mass action for forward reactions,

.

A constitutive relation for the specific reaction rate  must also be provided.

### Mass Action Reversible

According to the law of mass action for reversible reactions,



where  is a function that reduces to the equilibrium constant of the reversible reaction at chemical equilibrium (when ). Constitutive relations for the specific forward and reverse reaction rates,  and  respectively, must also be provided.

### Michaelis-Menten

Michaelis-Menten is a model for enzyme kinetics as represented by the reactions



where  is the enzyme,  is the substrate,  is the enzyme-substrate complex, and  is the product. The molar mass supply  producing  is related to the concentration of the substrate  via

,

where  is the maximum rate achieved by the system, at maximum (saturating) substrate concentrations.  is the substrate concentration at which the reaction rate is half of .

This relation may be derived by applying the law of mass action to the two reactions in . under the simplifying assumption that the reversible reaction between the enzyme and substrate reaches steady state much faster than the subsequent forward reaction forming the product. If the first and second reactions are denoted by subscripts 1 and 2, respectively, the law of mass action for the first (reversible) and second (forwar) reaction produces



The total enzyme concentration remains constant at , so that. If we now assume that the first reaction equilibrates much faster

than the second, then , in which case

,

where . Then,



where  represents the maximum value of , when . In practice, choosing  can produce the desired effect.

## Specific Reaction Rate

Specific reaction rate constitutive equations provide a relation for  as a function of solid matrix strain and the concentrations of solid-bound molecular species.

### Constant Specific Reaction Rate

For this material model,  is constant.

### Huiskes Remodeling

For this material, the specific reaction rate depends on the deviation of the specific strain energy from a threshold value,

,

where  is a constant,  is the strain energy density of the solid,  is the referential mass density of the solid,  is the threshold value for the specific strain energy. In this relation,  is evaluated from the solid deformation and  is evaluated from .

# Contact and Coupling

FEBio allows the user to connect the different parts of the model in various ways. Deformable parts can be connected to rigid bodies. Deformable objects can be brought in contact with each other. Rigid bodies can be connected with rigid joints. This chapter describes the different ways to couple parts together.

## Rigid-Deformable Coupling

In FEBio deformable bodies can be coupled with rigid bodies. The coupling requires a modification of the global stiffness matrix and residual vector. Additionally, degrees of freedom need to be introduced for the rigid bodies [[48](#_ENREF_48)]. This section describes the coupling between rigid and deformable bodies.

### Kinematics

The position vector **x** of a finite element node may be denoted as,

,

where **X** is the initial position of the node and **u** the displacement vector. If this node is connected to a rigid body the position can alternatively be written as,

,

where **r** is the current position of the center of mass of the rigid body and **a** is the relative position of the node to the center of mass. The vector **a** may be written in terms of its initial value  in the undeformed state and a rotation matrix,

.

In an incremental displacement formulation equation must be linearized:

,

where the linearization of the rotation matrix can be expressed in a more convenient form,

.

Here is and the matrix  is

.

For a model containing both deformable and rigid nodes the nodal degrees of freedom may be grouped, and the above expressions used to obtain a condensed set of unknowns:

.

Substituting this into the discrete form of the principle of virtual work yields expressions for the condensed finite element stiffness matrix and residual vector for the coupled rigid-deformable system:

.

Equation is now solved for the incremental update vector . The nodal positions of the deformable nodes can now be updated in the usual way.



Here, *k* is the iteration index of the Newon-Raphson iterations. The center of mass of the rigid body can now also be updated in a similar way.



To update the rotational degrees of freedom we employ quaternion algebra. The orientation of the rigid body at time *n+1* is represented by the (unit) quaternion . The rotational update vector  can be written as a quaternion as follows.



The updated orientation quaternion is then given by the quaternion product.



Finally, we must ensure that the updated quaternion is a unit quaternion. To accomplish this we normalize the quaternion.



Normalizing the quaternion guarantees that it represents a proper rotation.

### A single rigid body

The global system of equations can now be written as follows (for a single rigid body coupled to a deformable body),

.

Here is formed by adding all the residual vectors of all interface nodes that connect the deformable body to the rigid body,

,

where *i* sums over all interface nodes, and

.

It is recognized that  is simply the total residual force that is applied to the rigid body and is the total residual torque.

Constructing the stiffness matrix is accomplished in a similar manner. Assume *n* nodes per element, then the normal element stiffness matrix (in absence of rigid nodes) is given by,

,

where is the nodal stiffness matrix connecting node *i* to node *j*. These nodal stiffness matrices are now assembled into the global stiffness matrix. If node *i* and *j* are neither interface nodes their nodal stiffness matrix is assembled into in the usual manner,

,

where the sum now has to interpreted as the finite element assembly operator.

If node *j* is an interface node, than the nodal stiffness matrix gets assembled in the matrix:

.

If both nodes belong to the rigid body than the nodal element matrix gets assembled in as follows,

.

### Multiple Rigid Bodies

The previous results can easily be extended if there are multiple rigid bodies. The following section presents the approach for two rigid bodies, but the results can easily be generalized to *N* rigid bodies.

For two rigid bodies, the global system of equations takes the following form,

.

Care must be taken to assemble the nodal stiffness matrix in the correct global sub-matrix. If node *i* is not an interface node and node *j* is connected to rigid body 1, then their nodal stiffness matrix goes into . If, however, node *j* is attached to rigid body 2 then their nodal stiffness matrix goes into . If node *i* is connected to rigid body 1 and node *j* is connected to rigid body 2, then their nodal stiffness matrix goes into , and so on. Note that it is assumed here that a node may only connect to a single rigid body.

## Rigid Joints

A rigid joint is a location in space where two rigid bodies connect. The joint enforces a constraint on the system. This constraint can be written as,

.

Here is the location of the joint in the reference configuration and is the deformation map of rigid body *i*. Equation is a constraint equation that will be added to the total balance of virtual work.

.

Here, the ’s are the forces that will prevent the rigid bodies to separate at the joint position and . First we note that due to the third law of Newton , so that we can write the constraint term as,

.

Note that we can also write this as,

.

The constraint forces are determined by the augmented Lagrangian method and are given by,

,

where is the Lagrange multiplier and is a user defined penalty factor.

The linearization of is given by,



Using the rigid body assumption, the quantity can be written as follows,



And similarly for . If we now introduce the vectors,

.

Then we can write the constraint work as,

.

And the stiffness contribution as,

.

.

## Sliding Interfaces

This section summarizes the theoretical developments of the two body contact problem. After introducing some notation and terminology, the contact integral is presented, which contains the contribution to the virtual work equation from the contact tractions. Since the nonlinear contact problem is solved using a Newton based iterative method, the contact integral is linearized. Next, anticipating a finite element implementation, the contact integral and its linearization are discretized using a standard finite element approach. Finally the augmented Lagrangian method for enforcing the contact constraints is described.

### Contact Kinematics

For the most part the notation of this section follows [[49](#_ENREF_49)], with a few simplifications here and there since the implementation in FEBio is currently for quasi-static, frictionless, two body contact problem.

The volume occupied by body *i* in the reference configuration is denoted by where . The boundary of body *i* is denoted by and is divided into three regions , where is the boundary where tractions are applied, the boundary where the solution is prescribed and the part of the boundary that will be in contact with the other body. It is assumed that .

The deformation of body *i* is defined by . The boundary of the deformed body *i*, that is the boundary of is denoted by where is the boundary in the current configuration where the tractions are applied and similar definitions for and . See the figure below for a graphical illustration of the defined regions.



Figure 6‑1. The two-body contact problem.

Points in body 1 are denoted by **X** in the reference configuration and **x** in the current configuration. For body 2 these points are denoted by **Y** and **y**. To define contact, the location where the two bodies are in contact with each other must be established. If body 1 is the *slave body* and body 2 is the *master body*, then for a given point **X** on the slave reference contact surface there is a point on the master contact surface that is in some sense closest to point **X**. This closest point is defined in a closest point projection sense:

.

With the definition of established the *gap function* can be defined, which is a measure for the distance between **X** and ,

,

where is the local surface normal of surface evaluated at . Note that  when **X** has penetrated body 2, so that the constraint condition to be satisfied at all time is .

### Weak Form of Two Body Contact

The balance of linear momentum can be written for each of the two bodies in the reference configuration,

,

where is a weighting function and **P** is the 1st Piola-Kirchhoff stress tensor. The last term corresponds to the virtual work of the contact tractions on body *i*. For notational convenience, the notations and *w* are introduced to denote the collection of the respective mappings and (for *i=*1,2). In other words,



The variational principle for the two body system is the sum of for body 1 and 2 and can be expressed as,



Or in short,

.

Note that the minus sign is included in the definition of the contact integral . The contact integral can be written as an integration over the contact surface of body 1 by balancing linear momentum across the contact surface:

.

The contact integral can now be rewritten over the contact surface of body 1:

.

In the case of frictionless contact, the contact traction is taken as perpendicular to surface 2 and therefore can be written as, where is the (outward) surface normal andis to be determined from the solution strategy. For example in a Lagrange multiplier method the’s would be the Lagrange multipliers.

By noting that the variation of the gap function is given by

,

equation can be simplified as,

.

### Linearization of the Contact Integral

In a Newton-Raphson implementation the contact integral must be linearized with respect to the current configuration:

.

Examining the normal contact term first, the directional derivative of is given (for the case of the penalty regularization) by:



where is the penalty factor and is the Heaviside function. The quantity is given by,



### Discretization of the Contact Integral

The contact integral, which is repeated here,

,

will now be discretized using a standard finite element procedure. First it is noted that the integration can be written as a sum over the surface element areas:

,

where is the number of surface elements. The integration can be approximated using a quadrature rule,

,

where  are the number of integration points for element *e*. It is now assumed that the integration points coincide with the element’s nodes (e.g. for a quadrilateral surface element we have , ,  and ). With this quadrature rule, we have



so that,

.

If the following vectors are defined,



equation can then be rewritten as follows,

.

The specific form for will depend on the method employed for enforcing the contact constraint.

### Discretization of the Contact Stiffness

A similar procedure can now be used to calculate the discretized contact stiffness matrix. The linearization of the contact integral is repeated here:



Using matrix notation we can rewrite equation as,

,

where is as above and similar to  with replaced with  and ,



where,

.

The following vectors are also defined which depend on the vectors of :



where the matrix **A** is defined as,

.

Here, is the surface metric tensor and denotes the components of the surface curvature at .

### Augmented Lagrangian Method

The augmented Lagrangian method is used in FEBio to enforce the contact constraints to a user-specified tolerance. This implies that the normal contact tractions are given by,

.

Note that this assumption is consistent with the approach that was used in establishing the discretization of the linearization of the contact integral . In  is a penalty factor that is chosen arbitrarily.

The Newton-Raphson iterative method is now used to solve the nonlinear contact problem where Uzawa’s method (REF) is employed to calculate the Lagrange multipliers . This implies that the Lagrange multipliers are kept fixed during the Newton-Raphson iterations. After convergence the multipliers are updated and a new NR procedure is started. This procedure can be summarized by the following four steps.

1. **Initialize** the augmented Lagrangian iteration counter *k*, and the initial guesses for the multipliers:



1. **Solve** for , the solution vector corresponding to the fixed *k*th iterate for the multipliers,

,

where the contact tractions used to compute , the contact force, are governed by

.

1. **Update** the Lagrange multipliers and iteration counters:



1. **Return** to the solution phase.

Steps 2-4 of the above algorithm are generally repeated until all contact constraints are satisfied to a user-specified tolerance or little change in the solution vector from augmentation to augmentation is noted.

### Automatic Penalty Calculation

The determination of the penalty factor  can be a difficult task, since a good value may depend on both material parameters and geometrical factors. In FEBio the value of this penalty factor can be determined automatically. In this case FEBio will calculate a penalty factor for each facet using the following formula.

.

Here, is the effective bulk modulus, the surface area of the facet, the volume of the element to which this facet belongs and a user defined scale factor.

### Alternative Formulations

As of FEBio version 1.2, two alternative formulations for sliding contact are available. The first method, which is referred to as the *facet-to-facet sliding*, is very similar to the formulation described above. It only differs in that it uses a Gaussian quadrature rule instead of nodal integration. Because of the more accurate integration rule, it was noted that this method in many situations was more stable and resulted in better convergence.

The second alternative differs more significantly from the method described above. It also begins with the definition of a single contact integral over the slave surface.

.

But a different derivation is followed to obtain the linearization of this contact integral. The main reason for this difference is a subtly alternative definition for the gap function. In this method, it is defined as follows.

,

where, is the normal of the slave surface (opposed to the master normal as used in the derivation above). In this case, the point is no longer the closest point projection of **X** onto the master surface, but instead is the normal projection along . The linearization of equation now becomes,

.

Where, are the tangent vectors to the master surface at . Note that since is normal to the slave surface, equation does not reduce to equation .

In one assumes frictionless contact, the contact traction can be written as follows,

,

where, are the tangent vectors to evaluated at **X**. Using we can rewrite the contact integral as follows.

.

Where we assumed that the integration domain can be mapped to a 2D parametric domain, .

The linearization of now proceeds in the usual fashion. Omitting the details, it can be shown that the linearization of the contact integral results in,



where, and .

The discretization of the contact integral and its linearization now proceeds as usual. We will not derive the details, but it is important to point out that the resulting stiffness matrix for this particular contact formulation is not symmetric. Although this method has shown to give good results, especially in large compression problems, it was desirable to derive a symmetric version as well. Because of this, a slightly different formulation was also developed that does reduce to a symmetric stiffness matrix although this symmetric version did not seem to perform as well as the non-symmetric one.

## Biphasic Contact

### Contact Integral

See Section 5.6 for a review of biphasic materials, and [[50](#_ENREF_50)] for additional details on biphasic contact. The contact interface is defined between surfaces  and . Due to continuity requirements on the traction and fluxes, the external virtual work resulting from contact tractions  and solvent fluxes  (), may be combined into the contact integral



In the current implementation, only frictionless contact is taken into consideration, so that the contact traction has only a normal component, . To evaluate and linearize , define the covariant basis vectors on each surface as

,

where  represents the spatial position of points on , and  represent the parametric coordinates of that point. The unit outward normal on each surface is then given by

.

Now the contact integral may be rewritten as



and the linearization  of  has the form

.

### Gap Function

The gap function , representing the distance between the contact surfaces, is defined by

.

The linearization of variables associated with motion, pressure, and concentration, is given by



where



with  and .

### Penalty Method

Let the normal component of the contact traction be described by the penalty function,

,

where  is a penalty factor associated with . Similarly, let



where  is a penalty factor associated with . It follows that



Given these relations, it can be shown that the directional derivatives of the various terms appearing in the integrand of  are





where .

### Discretization

The contact integral may be discretized as

.

The variables may be interpolated over each element face according to



Then,



where



Similarly,



where







and



## Biphasic-Solute Contact

### Contact Integral

See Section 2.6 for a review of biphasic-solute materials. The contact interface is defined between surfaces  and . Due to continuity requirements on the traction and fluxes, the external virtual work resulting from contact tractions , solvent fluxes  and solute fluxes  (), may be combined into the contact integral



In the current implementation, only frictionless contact is taken into consideration, so that the contact traction has only a normal component, . To evaluate and linearize , define the covariant basis vectors on each surface as

,

where  represents the spatial position of points on , and  represent the parametric coordinates of that point. The unit outward normal on each surface is then given by

.

Now the contact integral may be rewritten as



and the linearization  of  has the form

.

### Gap Function

The gap function , representing the distance between the contact surfaces, is defined by

.

The linearization of variables associated with motion, pressure, and concentration, is given by



where



with  and .

### Penalty Method

Let the normal component of the contact traction be described by the penalty function,

,

where  is a penalty factor associated with . Similarly, let



and



where  and  are penalty factors associated with  and , respectively. It follows that



Given these relations, it can be shown that the directional derivatives of the various terms appearing in the integrand of  are







where .

### Discretization

The contact integral may be discretized as

.

The variables may be interpolated over each element face according to



Then,



where



Similarly,



where











and



## Tied Contact

In some situations it is useful to connect two non-conforming meshes together. This can be done by defining a tied contact interface. In FEBio, the tied contact works very similar to the sliding contact interface. We need to define a slave surface and a master surface, where it is assumed that the slave surface nodes will be tied to the master surface faces.

### Gap Function

Just as in sliding contact, we need to define a gap function that measures the distance between the slave and master surface. In order to do that, we first define the projection of a slave node to the master surface.

.

This definition is similar to that of the sliding interface, except that now the projection is done in the material reference frame. This implies that the projection only needs to be calculated once, at the beginning of the analysis. We can now proceed to the definition of the gap function.

.

An important observation is that the gap function is now a vector quantity since the gap needs to be closed in all direction, not just the normal direction as is the case in sliding contact.

### Tied Contact Integral

With the definition of the gap function at hand (equation ), we can define the contribution to the virtual work equation from the tied contact reaction forces.

.

Here, **T** is the reaction force that enforces the constraint . Since we anticipate the use of an augmented Lagrangian formalism, we can write this reaction force as follows.

.

The vector quantity is the Lagrangian multiplier and is a penalty factor.

### Linearization of the Contact Integral

Since equation is nonlinear we need to calculate the linearization. For tied contact, this is simply given by the following equation.

.

Where



and

.

We also introduced the notation .

The discretization of will lead to a contribution to the stiffness matrix. Notice that due to symmetry between and this matrix will be symmetric.

### Discretization

The contact integral can be discretized as follows. First, we split the integration over all the slave surface elements.

.

The integration can be approximated by a quadrature rule,

.

If we use a nodally integrated elements, we have



so that,

.

We can now write the contact integral in its final form,

,

where

,

,

and

.

For the linearized tied contact integral , a similar discretization procedure leads to,

,

where

.

# Dynamics

FEBio can perform a nonlinear dynamic analysis by iteratively solving the following nonlinear semi-discrete finite element equations [REF BATHE].



Here, **M** is the mass matrix, **K** the stiffness matrix, **T** the internal force (stress) vector and **F** the externally applied loads. The upperscript index *k* refers to the iteration number, the subscript *n* refers to the time increment. The trapezoidal (or midpoint) rule is used to perform the time integration. This results in the following approximations for the displacement and velocity updates.



Using we can solve for  .



Substituting this into equation results in the following linear system of equations.



Solving this equation for  and using gives the new displacement vector  . The acceleration vector  can then be found from and the velocity vector  from. This algorithm is repeated until convergence is reached.

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1. Note that weights sum up to one and not to the volume of the tet in the natural coordinate system (i.e. 1/6). [↑](#footnote-ref-1)