SIGGRAPH 2012 Course

FEM Simulation of 3D Deformable Solids: A practitioner's guide to theory, discretization and model reduction.

Part One:

The classical FEM method and discretization methodology

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Chapter 1

Preface

Simulation of deformable elastic solids has evolved into a popular tool for visual effects, games and interactive virtual environments. The Finite Element Method has been very popular in this context, especially in applications that can benefit from its versatility in representing elastic bodies with intricate geometric features and diverse material properties. Techniques for solids simulation that have been broadly used in graphics draw upon a rich, decades-long literature in Galerkin methods, discrete elliptic PDEs and continuum mechanics theory. As many of these techniques originated in theoretical and engineering disciplines other than graphics and visual computing, it may be somewhat challenging for a practitioner with modest theoretical exposure or familiarity with these fields to navigate some of the most established mechanical engineering or computational physics reference textbooks, especially if their goal is to acquire a high-level understanding of the basic tools needed for implementing a simulation system. This document aims to provide a concise, yet lightweight synopsis of the relevant theory, with adequate attention to implementation details from the perspective of a graphics developer. Most of the material referenced in these notes resulted from the author's long and rewarding interactions with graduate students at Stanford, UCLA and UW-Madison, as well as the experience of the graduate class "Introduction to physics-based modeling and simulation" offered at the University of Wisconsin.

This document assumes minimal to no exposure to continuum mechanics or finite element discretizations. However, a particular flavor of calculus background is presumed, including:

- Familiarity with functions of several variables, partial derivaties, volume and surface integrals.

- Some exposure to numerical techniques for solving linear systems of equations, and the Newton-Raphson method for finding approximate solutions to nonlinear problems.

- A good understanding of linear algebra, including concepts such as vectors, matrices and (higher-order) tensors. Familiarity with determinants, eigenvalue problems and the Singular Value Decomposition is also assumed.
- Although many of the proofs and derivations are treated as optional reading, the majority of them make heavy use of *differentials* (linearized tensors) and reference complex differentiation concepts (such as the derivative of a matrix function with respect to a matrix argument).

As a supplement to the present introduction to FEM methods for deformable solids simulation, the following textbooks are highly recommended:

J. Bonet and R. Wood, *Nonlinear continuum mechanics for Finite Element Analysis*, (2nd ed.), Cambridge University Press

O. Gonzalez and A. Stuart, *A first course in Continuum Mechanics*, Cambridge University Press

T. Hughes, *The Finite Element Method: Linear Static and Dynamic Finite Element Analysis*, Dover Publications

T. Belytschko, W. Lui and B. Moran, *Nonlinear Finite Elements for Continua and Structures*, Wiley

J. Simmonds, *A Brief on Tensor Analysis*, (2nd ed.), Springer-Verlag

G. Golub and C. van Loan, *Matrix Computations*, (3rd ed.), Johns Hopkins University Press

J. Demmel, *Applied Numerical Linear Algebra*, SIAM

Text in shaded boxes presents theoretical proofs, provides examples or provides further insight on the preceding topics. This content can be treated as optional reading, and omitting it should not compromise the understanding of subsequent topics.

Chapter 2

Elasticity in three dimensions

In this chapter we focus on three-dimensional elastic bodies deforming in space, and discuss how we can formulate quantitative descriptions for the deformed shape of an object and the forces resulting from it. To a certain extent, these formulations are analogous to similar concepts from mass-spring systems, or deformable elastic strands. However, since a volumetric body is able to alter its shape in more complex ways than, for example, a one-dimensional elastic strand, many concepts that may be familiar from simpler mechanical systems will need to be extended and become more expressive. For the time being, and until chapter 4, we will not concern ourselves with discretization issues. Our discussion will focus on the continuous phenomenon of elastic deformation, as if we had infinite resolution at our disposal.

2.1 Deformation map and deformation gradient

Our initial objective is to provide a concise mathematical description of the deformation that an elastic body has sustained. This formulation will lay the foundation for appropriate representations of other physical properties such as force and energy. We begin by placing the undeformed elastic object in a coordinate system, and denote by Ω the volumetric domain occupied by the object. This domain will be referred to as the *reference (or undeformed) configuration*, and we follow the convention that capital letters $\vec{X} \in \Omega$ are used when referring to individual material points in this undeformed shape. Note that the precise position and orientation of the undeformed elastic body within the reference space is not important and can be chosen at will, as long as the shape of the object corresponds to a rest configuration.

When the object undergoes deformation, every material point $\vec{X}$ is being displaced to a new *deformed* location as seen in figure 2.1 (top) which is, by convention, denoted by a lowercase variable $\vec{x}$. The relation between each material point and its respective deformed location is captured by the *deformation function* $\vec{\phi} : \mathbf{R}^3 \to \mathbf{R}^3$ which maps every material point $\vec{X}$ to its respective deformed location $\vec{x} = \vec{\phi}(\vec{X})$.

In some cases we also use the notation: $\vec{X} = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}$

An important physical quantity derived directly from $\vec{\phi}(\vec{X})$, whose utility will become apparent in the next sections, is the *deformation gradient* tensor $\mathbf{F} \in \mathbf{R}^{3\times 3}$. If we write $\vec{X} = (X_1, X_2, X_3)^T$ and $\vec{\phi}(\vec{X}) = \Big(\phi_1(\vec{X}), \phi_2(\vec{X}), \phi_3(\vec{X})\Big)^T$ for the three components of the vector-valued function $\vec{\phi}$, the deformation gradient is written as:

$$\mathbf{F} := \frac{\partial(\phi_1, \phi_2, \phi_3)}{\partial(X_1, X_2, X_3)} = \begin{pmatrix} \partial\phi_1/\partial X_1 & \partial\phi_1/\partial X_2 & \partial\phi_1/\partial X_3 \\ \partial\phi_2/\partial X_1 & \partial\phi_2/\partial X_2 & \partial\phi_2/\partial X_3 \\ \partial\phi_3/\partial X_1 & \partial\phi_3/\partial X_2 & \partial\phi_3/\partial X_3 \end{pmatrix}$$

or, in index notation $F_{ij} = \phi_{i,j}$. That is, $\mathbf{F}$ is the Jacobian matrix of the deformation map. Note that, in general, $\mathbf{F}$ will be spatially varying across Ω; in the next sections we will use the notation $\mathbf{F}(\vec{X})$ if such dependence needs to be made explicit.

Simple examples of deformation fields

The deformation depicted in the top row of figure 2.1 is indicative of arbitrary shape changes that are likely to occur in animation tasks. For such instances of deformation it would not be possible to write $\phi(\vec{X})$ in closed form, and simulation would be employed instead to generate a numerical approximation. We can provide, however, some intuitive closed-form expressions for certain simple examples of deformation scenarios:

- Figure 2.1(a) depicts a configuration change which is merely a constant translation, say, by a vector $\vec{t}$. Here, the deformation map and gradient are:
$$\vec{x} = \phi(\vec{X}) = \vec{X} + \vec{t} \qquad \mathbf{F} = \partial\phi(\vec{X})/\partial\vec{X} = \mathbf{I}$$
- Figure 2.1(b) illustrates a scaling by a constant factor γ, specifically in our case a dilation by $\gamma = 1.5$. depicts a configuration change which is merely a constant translation, say, by a vector $\vec{t}$. In this case, we have:
$$\phi(\vec{X}) = \gamma\vec{X} \qquad \mathbf{F} = \gamma\mathbf{I}$$
- In figure 2.1(c) the reference shape has been scaled along the horizontal axis by a factor of 0.7, where the vertical axis is stretched by a factor of 2. Thus:
$$\begin{pmatrix} x \\ y \end{pmatrix} = \phi(\vec{X}) = \phi\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} 0.7X \\ 2Y \end{pmatrix} \qquad \mathbf{F} = \begin{pmatrix} 0.7 & 0 \\ 0 & 2 \end{pmatrix}$$
- The configuration of figure 2.1(d) is the result of a 45° counter-clockwise rotation around the origin. Therefore, we have:
$$\begin{pmatrix} x \\ y \end{pmatrix} = \phi(\vec{X}) = \begin{pmatrix} \cos 45^\circ & -\sin 45^\circ \\ \sin 45^\circ & \cos 45^\circ \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} \qquad \mathbf{F} = \begin{pmatrix} \cos 45^\circ & -\sin 45^\circ \\ \sin 45^\circ & \cos 45^\circ \end{pmatrix}$$

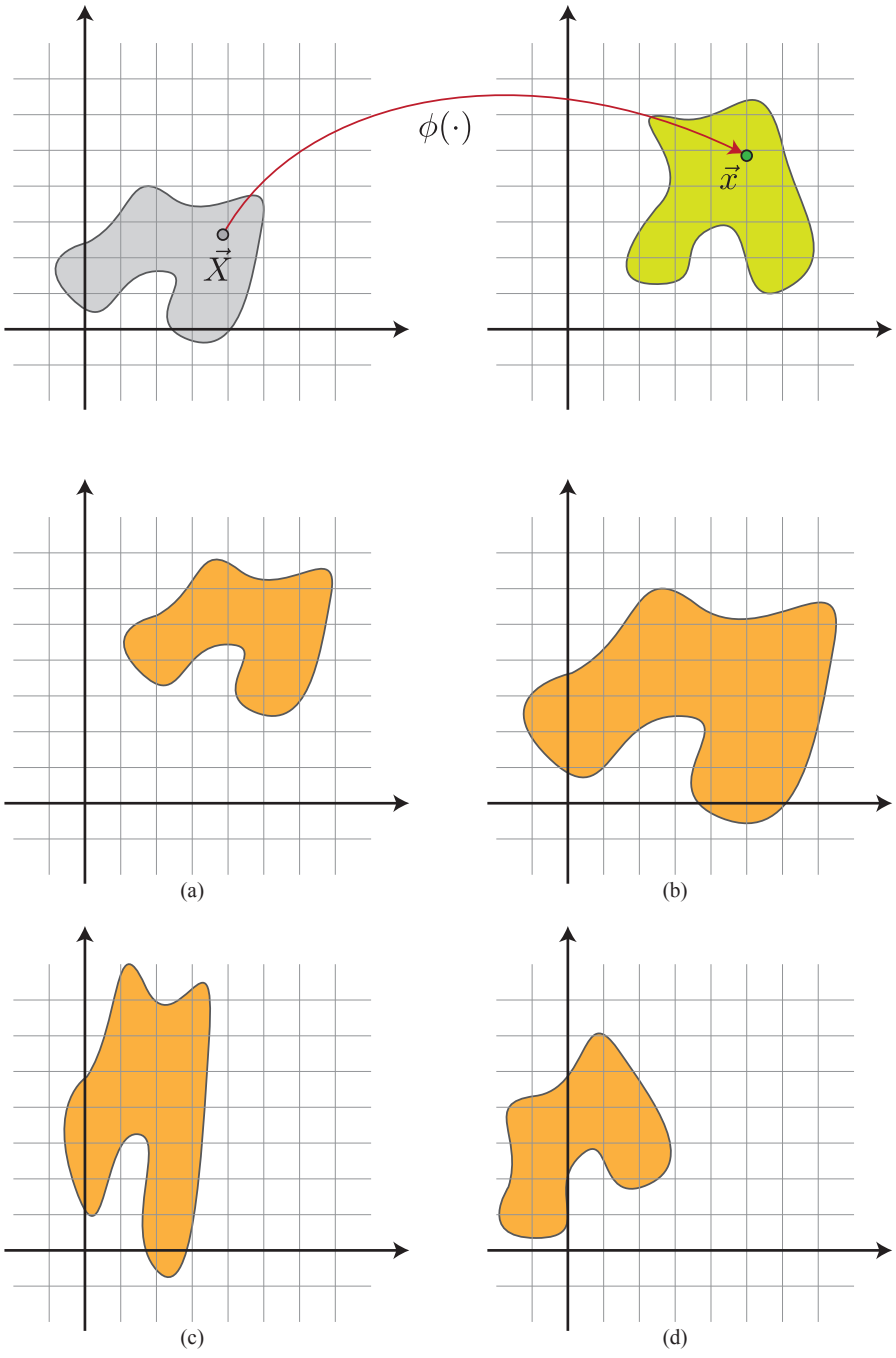

Figure 2.1: Top row: Illustration of the deformation map ϕ from the reference configuration (left) to the deformed shape (right). Bottom two rows: Sample deformations of (a) translation, (b) uniform scaling, (c) anisotropic scaling, (d) rotation.

2.2 Strain energy and hyperelasticity

One of the consequences of elastic deformation is the accumulation of potential energy in the deformed body, which is referred to as *strain energy* in the context of deformable solids. We use the notation $E[\phi]$ for the strain energy, which suggests that the energy is fully determined by the deformation map of a given configuration. However intuitive, this statement nevertheless reflects a significant hypothesis that led to this formulation: we have assumed that the potential energy associated with a deformed configuration only depends on the final deformed shape, and not on the deformation path over time that brought the body into its current configuration. The independence of the strain energy on the prior deformation history is a characteristic property of so-called *hyperelastic* materials (which is the only class of materials we will address in this course). This property of is closely related with the fact that elastic forces of hyperelastic materials are *conservative*: the total work done by the internal elastic forces in a deformation path depends solely on the initial and final configurations, not the path itself.

Different parts of a deforming body undergo shape changes of different severity. As a consequence, the relation between deformation and strain energy is better defined on a local scale. We achieve that by introducing an *energy density* function $\Psi[\phi; \vec{X}]$ which measures the strain energy *per unit undeformed volume* on an infinitesimal domain dV around the material point $\vec{X}$. We can then obtain the total energy for the deforming body by integrating the energy density function over the entire domain Ω:

$$E[\phi] = \int_\Omega \Psi[\phi; \vec{X}] d\vec{X}$$

Let us focus on a specific material location $\vec{X}_*$. Since the energy density $\Psi[\phi; \vec{X}_*]$ would only need to reflect the deformation behavior in an infinitesimal neighborhood of $\vec{X}_*$, we can reasonably approximate the deformation map in this tiny region using a first-order Taylor expansion:

$$\begin{aligned}\phi(\vec{X}) &\approx \phi(\vec{X}_*) + \left.\frac{\partial \phi}{\partial \vec{X}}\right|_{\vec{X}_*} (\vec{X} - \vec{X}_*) = \vec{x}_* + \mathbf{F}(\vec{X}_*)(\vec{X} - \vec{X}_*) \\ &= \underbrace{\mathbf{F}(\vec{X}_*)}_{\mathbf{F}_*} \vec{X} + \underbrace{\vec{x}_* - \mathbf{F}(\vec{X}_*)\vec{X}_*}_{\vec{t}} = \mathbf{F}_* \vec{X} + \vec{t}\end{aligned}$$

This equation suggests that $\Psi[\phi; \vec{X}_*]$ should be expressible as a function of $\mathbf{F}_*$ and $\vec{t}$, as these values fully parameterize the local Taylor approximation of ϕ near $\vec{X}_*$. Furthermore, we can expect that the value of the vector $\vec{t}$ would be irrelevant in this expression: different values of this parameter would indicate deformations that differ only by a constant translation, thus producing the same deformed shape and the same strain energy. Thus, we expect that the energy density function should be

expressible as $\Psi[\phi; \vec{X}] = \Psi(\mathbf{F}(\vec{X}))$, i.e. a function of the local deformation gradient alone.

The previous arguments have simply established that the energy density function is expected to be a function of the deformation gradient. However, we have not provided specific formulas for $\Psi(\mathbf{F})$. This is intentional as we want the flexibility to accommodate a variety of materials. Ultimately, the precise mathematical expression for $\Psi(\mathbf{F})$ will be the defining property of the material modeled.

What would a formula for $\Psi(\mathbf{F})$ look like?

Chapter 3 will provide concrete examples of material models and their associated energy definitions. For the time being we list a few examples of (largely academic and oversimplified) hypothetical materials. A naturally expected property is that the energy is bounded from below, thus minimum-energy states exist where the deforming object can settle to. For example:

$$\Psi(\mathbf{F}) = \frac{k}{2}\|\mathbf{F}\|_F^2 \qquad \text{where } k > 0.$$

This is an interesting hypothetical scenario. We would describe it as a "zero rest-volume material" in analogy to a "zero rest-length spring": The minimum energy is attained when $\mathbf{F} = \mathbf{0}$ throughout Ω, which means that $\phi(\vec{X}) = \text{const}$, i.e. all material points have the natural tendency to collapse down to a single point location. Although such a material might be useful for “glueing” tasks, akin to zero rest-length springs, it is unnatural in the sense that the *reference* configuration Ω is not an *equilibrium* configuration. In order to preserve such a property, we would expect that when $\mathbf{F} = \mathbf{I}$, corresponding to an undeformed scenario $\phi(\vec{X}) = \vec{X}$, would be a minimum of the energy. This could be achieved by setting:

$$\Psi(\mathbf{F}) = \frac{k}{2}\|\mathbf{F} - \mathbf{I}\|_F^2 \qquad \text{where } k > 0.$$

This model will have minimum energy when the object is in its reference configuration, or a constant translation away from it. Unfortunately, this model would not treat a *rotation* of the undeformed shape as a rest configuration, and the energy would be nonzero in this case. This lack of *rotational invariance* serves as motivation for the material models in the later sections of chapter 3.

2.3 Force and traction

The next physical concept to be addressed is the elastic *force* incurred by a given deformation. First, consider a simple case from elementary mechanics: a small body

(ideally dimensionless, i.e. a point mass) moving in a conservative force field. An easy example would be the gravitational field, where a body located at $\vec{x} = (x, y, z)$ has potential energy $E(\vec{x}) = m\vec{G} \cdot \vec{x} = mgz$, where $\vec{G} = (0, 0, g)$ is the acceleration of gravity (the z-axis is assumed to be vertical). We can then obtain the gravitational force as the negative gradient of the potential energy with respect to the object position $\vec{x}$:

$g = 9.81 m/s^2$

$$\vec{f} = -\frac{\partial E(\vec{x})}{\partial \vec{x}} = (0, 0, -mg)$$

However, when attempting to express a similar relation between force and energy for deformable bodies we need to be cautious of the fact that, in the absence of a prior discretization, such bodies form a continuous distribution of material, rather than a collection of isolated point masses. As a consequence, the appropriate quantitative description for elastic forces resulting from deformation would also be via a distribution. Thus, we use $\vec{f}(\vec{X})$ to denote force density, or more specifically *force per unit undeformed volume*, in an infinitesimal region around $\vec{X}$. The aggregate force on a finite region $A \subset \Omega$ would then be computed by integrating

$$\vec{f}_{\text{aggregate}}(A) = \int_A \vec{f}(\vec{X}) d\vec{X}. \tag{2.1}$$

Unfortunately, this description is not appropriate for the force exerted by the body *along its boundary*. Consider an elastic body which is uniformly compressed (e.g. $\phi(\vec{X}) = \alpha\vec{X},\ \alpha < 1$) to a lower volume. We would expect the body to react by pushing back against the apparatus that is causing the compression, and this restorative force would act along the surface of contact $S \subset \partial\Omega$. This time we define the *traction* $\vec{\tau}(\vec{X})$ to be the (surface) force density function that measures the *force per unit undeformed area* along an infinitesimal region of the boundary surface $\vec{X}$. Once again, the aggregate force on a finite boundary region $B \subset \partial\Omega$ is computed by integrating:

$$\vec{f}_{\text{aggregate}}(B) = \oint_B \vec{\tau}(\vec{X}) dS. \tag{2.2}$$

Why treat (interior) force density and (boundary) traction separately? Ultimately, don't both of them just refer to standard elastic forces?

In loose terms, the reason is that on a force-per-volume basis, the net elastic force is quantitatively "stronger" on the boundary than on the interior; the force density would generally be a bounded function on the interior, but might look like a Dirac delta function on the boundary. This makes it possible to have a nonzero aggregate force along boundary patches, even though those would have had zero volume in an

integral such as (2.1). Instead of dealing with the peculiarities of integrating Delta functions just for the sake of having a single "force-per-unit-volume" descriptor, it makes better practical sense to separate force computation into the interior term of equation (2.1) and the boundary term of equation (2.2), where the integrands in either case are regular, finite-valued functions.

The question that remains is: how is it physically meaningful for elastic forces to have this apparent greater strength at the boundary? The important observation here is that $\vec{f}(\vec{X})$ is the total force that a point $\vec{X}$ receives from its surrounding material, *from all directions*. Although the force exceeded along each individual direction might be substantial, significant cancellation is to be expected when the force contributions of all directions are added up. For example, if we stretch a homogeneous material uniformly, each deformed material point will receive strong, yet equal (in magnitude) attractive forces along each direction, leading to a zero net force. Boundary points, on the other hand, only receive an elastic response from their material side, making it easier to accumulate a larger net force.

Finally, it is important to note that the distinction between force density and traction largely goes away once a discrete representation of the deformable body is adopted. In such case, we use *nodal forces* (instead of densities) as descriptors of the elastic material response, and their treatment is practically identical regardless of whether they reside on the boundary or interior of the deforming body.

2.4 The First Piola-Kirchhoff stress tensor

The differences between interior force density and boundary traction suggest that neither concept is fundamental enough to describe all aspects of the elastic response of deforming bodies. There is, however, a fundamental force descriptor that both such quantities can be derived from: the *stress tensor*. There is a variety of "stress" descriptors that can be used for this purpose; for our discussion, we will focus on the *1st Piola-Kirchhoff stress tensor* $\mathbf{P}$, a 3×3 matrix with the following properties:

- The internal traction at a boundary location $\vec{X} \in \partial\Omega$ is given by

$$\vec{\tau}(\vec{X}) = -\mathbf{P} \cdot \vec{N} \tag{2.3}$$

  where $\vec{N}$ is the outward pointing unit normal to the boundary *in the reference (undeformed) configuration*. This can serve as a formal definition for the stress tensor $\mathbf{P}$: for any interior point $\vec{X} \in \Omega \setminus \partial\Omega$ we can hypothetically slice the material with a cut through $\vec{X}$ and perpendicular to $\vec{N}$, and compute the traction along such a cut. Then, $\mathbf{P}$ would be the unique matrix that relates $\vec{\tau}$ and $\vec{N}$ as in equation (2.3) for all possible boundary orientations.

- The internal force density can also be computed from $\mathbf{P}$, as follows:

$$\vec{f}(\vec{X}) = \mathbf{div}_{\vec{X}}\mathbf{P}(\vec{X}), \quad \text{or component-wise:} \quad f_i = \sum_{j=1}^{3} P_{ij,j} = \frac{\partial P_{i1}}{\partial X_1} + \frac{\partial P_{i2}}{\partial X_2} + \frac{\partial P_{i3}}{\partial X_3}.$$

  We emphasize that the divergence operator and/or its component derivatives are taken with respect to the *undeformed/reference* coordinates $\vec{X}$.

- For hyperelastic materials, $\mathbf{P}$ is purely a function of the deformation gradient, and is related to the strain energy via the simple formula:

$$\mathbf{P}(\mathbf{F}) = \partial\Psi(\mathbf{F})/\partial\mathbf{F}$$

As described, the 1st Piola-Kirchhoff stress tensor can be used to yield formulas both for force and tension, and is readily computed from the strain energy density definition. In fact, there are two equally popular (and, in fact, equivalent) ways to describe the material properties of a hyperelastic material: (a) an explicit formula for Ψ as a function of $\mathbf{F}$, or (b) an explicit formula for $\mathbf{P}$ as a function of $\mathbf{F}$. We will provide both types of definitions for all materials discussed in in this document.

Example

In section 2.2 we listed a hypothetical hyperelastic material with energy density $\Psi(F) = (k/2)\|\mathbf{F} - \mathbf{I}\|_F^2$. We are now in a position to give quantitative descriptions for the force and traction such a model would generate in response to deformation.

The Piola stress is computed as follows

$$\delta\Psi(F) = (k/2)\delta\left[(\mathbf{F}-\mathbf{I}):(\mathbf{F}-\mathbf{I})\right] = k(\mathbf{F}-\mathbf{I}):\delta\mathbf{F} = \frac{\partial\Psi}{\partial\mathbf{F}}:\delta\mathbf{F}$$

$$\text{thus} \quad \mathbf{P} = \partial\Psi/\partial\mathbf{F} = k(\mathbf{F}-\mathbf{I}), \quad \text{or component-wise:} \quad P_{ij} = k(\phi_{i,j} - \delta_{ij})$$

From this, internal forces are computed as

$$f_i = \textstyle\sum_j P_{ij,j} = \sum_j k\phi_{i,jj} = k\Delta\phi_i \Rightarrow \vec{f} = k\Delta\vec{\phi}$$

Given such a material and appropriate boundary conditions, a rest configuration would be found by solving $\vec{f} = \vec{0}$ (in the absence of external forces) or $\Delta\vec{\phi} = \vec{0}$.

Lastly, let us assume a uniform expansion by a function of 2. Thus $\phi(\vec{X}) = 2\vec{X}$, $\mathbf{F} = 2\mathbf{I}$, and $\mathbf{P} = k\mathbf{I}$. The traction that would result from this stress on a surface perpendicular to $\vec{N}$ would be $\vec{\tau} = -k\vec{N}$ (generating boundary forces that trigger inwards motion to restore the original shape and volume).

We note that in much of the relevant literature, a different notational convention is followed where $\vec{f}$ and $\vec{\tau}$ refer to the *externally applied* force density and traction, respectively. The relation between these quantities and stress is then expressed by assuming that the body is in an equilibrium configuration, where such externally applied forces and tractions balance out exactly the internal elastic force and traction. The equations obtained under this convention would be:

$$\vec{f} + \mathbf{div}\mathbf{P} = 0, \quad \text{and} \quad \vec{\tau} = \mathbf{P} \cdot \vec{N}.$$

In this document, we will retain our original definition where $\vec{f}$ and $\vec{\tau}$ refer to internal forces, along with their respective relations to $\mathbf{P}$ from earlier in this section, as these formulas hold true even if the deforming body is not in an equilibrium configuration. In cases where we need to refer to any externally applied force or traction we will use symbols $\vec{f}_{\text{ext}}$ and $\vec{\tau}_{\text{ext}}$, instead.

We provide a brief justification for the formulas relating the Piola stress $\mathbf{P}$ to force and traction. The intent of the derivations that follow is not to give a rigorous proof, but rather to explain the thought process that gave rise to these definitions.

Consider an arbitrary deformation $\vec{x} = \vec{\phi}(\vec{X})$, and a small perturbation $\delta\vec{\phi}(\vec{X})$ away from it. As the deforming body transitions from configuration $\vec{\phi}$ to the nearby configuration $\vec{\phi}+\delta\vec{\phi}$ the strain energy will be reduced by a certain amount δE equal to the work done by the elastic forces:

$$\delta E = -\int_\Omega \vec{f}(\vec{X}) \cdot \delta\vec{\phi}(\vec{X}) d\vec{X} - \oint_{\partial\Omega} \vec{\tau}(\vec{X}) \cdot \delta\vec{\phi}(\vec{X}) dS. \tag{2.4}$$

Note that the work is separately integrated in the interior and boundary regions, due to the quantitative difference of force and traction. The change in strain energy can also be expressed as:

$$\delta E = \delta\left[\int_\Omega \Psi(\mathbf{F}) d\vec{X}\right] = \int_\Omega \delta\left[\Psi(\mathbf{F})\right] d\vec{X} = \int_\Omega \left[\frac{\partial\Psi}{\partial\mathbf{F}} : \delta\mathbf{F}\right] d\vec{X} = \int_\Omega \left[\mathbf{P} : \delta\mathbf{F}\right] d\vec{X}$$
$$= \sum_{i,j=1}^{3} \int_\Omega P_{ij}\delta F_{ij} d\vec{X} = \sum_{i,j=1}^{3} \int_\Omega P_{ij} \cdot \frac{\partial}{\partial X_j}\left[\delta\phi_i(\vec{X})\right] d\vec{X}$$

Using integration by parts, this is equivalently written as

$$\delta E = \sum_{i,j=1}^{3} \left[-\int_\Omega \frac{\partial}{\partial X_j}\left[P_{ij}\right] \cdot \delta\phi_i(\vec{X}) d\vec{X} + \oint_{\partial\Omega} P_{ij}N_j \cdot \delta\phi_i(\vec{X}) d\vec{X}\right]$$
$$= -\int_\Omega \mathbf{div}\mathbf{P} \cdot \delta\vec{\phi}(\vec{X}) d\vec{X} + \oint_{\partial\Omega} (\mathbf{P} \cdot \vec{N}) \cdot \delta\vec{\phi}(\vec{X}) d\vec{X} \tag{2.5}$$

$$\vec{N} = \begin{pmatrix} N_1 \\ N_2 \\ N_3 \end{pmatrix}$$

From equations (2.4, 2.5) and using the fundamental lemma of variational calculus we have that $\vec{f}(\vec{X}) = \mathbf{div}\mathbf{P}$, and $\vec{\tau}(\vec{X}) = -\mathbf{P}\vec{N}$.

Chapter 3

Constitutive models of materials

In this section we survey a number of different simulated materials and describe how their physical properties are encoded in their respective governing equations. The mathematical description of the physical traits of a given material is referred to as its *constitutive model* and includes the equations that relate stimuli (e.g. deformations) to the material response (e.g. force, stress, energy) they trigger. In the spirit of the preceding chapter, two possibilities for what a *constitutive equation* can be are given by the formula for the Piola stress $\mathbf{P}$ as a function of the deformation gradient $\mathbf{F}$, or the formula for the energy density Ψ as a function of $\mathbf{F}$. For simplicity, we will focus on *isotropic* materials, whose response to deformation is independent of the orientation that such deformation is applied in.

3.1 Strain measures

In principle, an explicit formula that relates Ψ and $\mathbf{F}$ (or $\mathbf{P}$ and $\mathbf{F}$) would be perfectly adequate as a constitutive equation: think of the formula $\Psi(\mathbf{F}) = \|\mathbf{F}-\mathbf{I}\|_F^2$ from the previous chapter as an example of this fact. The challenge, however, with designing constitutive models in this fashion is that using the raw elements of the matrix $\mathbf{F}$ can be a very unintuitive way to argue about the flavor and severity of a given deformation. Perhaps a certain material's response is dominated by its affinity for volume conservation, while a different material might prioritize resistance to shear. One would imagine that metrics such as "the ratio of volumetric expansion" or "the shear angle" would be much more effective in expressing the severity of the types of deformation that are most relevant to such materials. As a consequence, it is common for the design process for constitutive models to define certain intermediate quantities (examples of which are *strain measures* and *invariants*, discussed in this chapter) which are derived from $\mathbf{F}$, yet capture the specific traits of the deformation that the energy or stress values depend on more concisely than the deformation gradient itself.

A *strain measure* is intended to be a quantitative descriptor for the severity of a given deformation, i.e. a way to gauge how far this configuration is from a *rest configuration*. For this reason, although strain measures are derived from the deformation gradient, they strive to retain as much information from it that is relevant to assessing deformation magnitude while disregarding any information contained in it that is unrelated to shape change. Consider the *Green strain tensor* $\mathbf{E} \in \mathbf{R}^{3\times3}$, defined as:

$$\mathbf{E} = \frac{1}{2}\left(\mathbf{F}^T\mathbf{F} - \mathbf{I}\right). \tag{3.1}$$

The Green strain tensor exemplifies many of the properties that we would ask for in a strain measure. When the body is in its reference configuration, i.e. $\vec{\phi}(\vec{X}) = \vec{X}$, we have $\mathbf{F} = \mathbf{I}$ and thus $\mathbf{E} = \mathbf{0}$. The Green strain would also be zero if the elastic body is merely rotated and translated from its reference position, without changing its shape; in such a case $\vec{\phi}(\vec{X}) = \mathbf{R}\vec{X} + \vec{t}$ (where $\mathbf{R}$ is a rotation matrix), thus $\mathbf{F} = \mathbf{R}$ and $\mathbf{E} = \mathbf{0}$ since $\mathbf{R}^T\mathbf{R} = \mathbf{I}$.

More generally, even for non-rigid motions, the deformation gradient can be decomposed as $\mathbf{F} = \mathbf{RS}$ into the product of a rotation matrix $\mathbf{R}$, and a symmetric factor $\mathbf{S}$ via the polar decomposition. As a 3D rotation matrix $\mathbf{R}$ encapsulates three degrees of freedom, while the symmetric $\mathbf{S}$ has 6 independent degrees of freedom. Substituting the polar decomposition into equation (3.1) we obtain:

$$\mathbf{E} = \frac{1}{2}\left(\mathbf{S}^2 - \mathbf{I}\right).$$

Thus, the Green strain succeeds in discarding the rotational degrees of freedom, which have no bearing on the severity of deformation, and retains the stretch/shear information in the 6-DOF symmetric factor $\mathbf{S}$. This is also accomplished without explicitly forming the polar decomposition.

The price one has to pay for the useful properties the Green strain offers, is that the expression of equation (3.1) is a nonlinear (quadratic) function of deformation. This increases the complexity of constitutive models that are constructed based on it and, as we will see next, will lead to discretizations with nodal forces being nonlinear functions of nodal positions. In an effort to remedy this, we construct a *linear* approximation of equation (3.1) by forming a Taylor expansion around the undeformed configuration $\mathbf{F} = \mathbf{I}$.

$$\mathbf{E}(\mathbf{F}) \approx \underbrace{\mathbf{E}(\mathbf{I})}_{=\mathbf{0}} + \left.\frac{\partial \mathbf{E}}{\partial \mathbf{F}}\right|_{\mathbf{F}=\mathbf{I}} : (\mathbf{F} - \mathbf{I})$$

The derivative $\partial\mathbf{E}/\partial\mathbf{F}$ is most conveniently defined via the differential $\delta\mathbf{E}$:

$$\frac{\partial \mathbf{E}}{\partial \mathbf{F}} : \delta\mathbf{F} = \delta\mathbf{E} = \frac{1}{2}\left(\delta\mathbf{F}^T\mathbf{F} + \mathbf{F}^T\delta\mathbf{F}\right)$$

Thus

$$\left.\frac{\partial \mathbf{E}}{\partial \mathbf{F}}\right|_{\mathbf{F}=\mathbf{I}} : (\mathbf{F}-\mathbf{I}) = \frac{1}{2}\left[(\mathbf{F}-\mathbf{I})^T\mathbf{I} + \mathbf{I}^T(\mathbf{F}-\mathbf{I})\right] = \frac{1}{2}\left(\mathbf{F}+\mathbf{F}^T\right) - \mathbf{I}$$

The matrix resulting from this linear approximation of $\mathbf{E}(\mathbf{F})$ is denoted by $\boldsymbol{\epsilon}$, where:

$$\boldsymbol{\epsilon} = \frac{1}{2}\left(\mathbf{F}+\mathbf{F}^T\right) - \mathbf{I}$$

and called the *small strain tensor*, or the *infinitesimal strain tensor*. This strain tensor will give rise to a computationally lightweight constitutive model called *linear elasticity*, described in the next section, and enable discretizations which have a linear mapping between nodal positions and nodal elastic forces. As expected, this convenience comes with a certain limitation: the small strain tensor can be considered a reliable measure of deformation for *small* motions only (hence the name) while pronounced artifacts will occur if used in a large deformation scenario.

3.2 Linear elasticity

The simplest practical constitutive model is *linear elasticity*, defined in terms of the strain energy density as:

$$\Psi(\mathbf{F}) = \mu\boldsymbol{\epsilon}:\boldsymbol{\epsilon} + \frac{\lambda}{2}\mathrm{tr}^2(\boldsymbol{\epsilon}) \tag{3.2}$$

where $\boldsymbol{\epsilon}$ is the small strain tensor and μ, λ are the *Lamé coefficients*, which are related to the the material properties of *Young's modulus* k (a measure of stretch resistance) and *Poisson's ratio* ν (a measure of incompressibility) as:

$$\mu = \frac{k}{2(1+\nu)} \qquad \lambda = \frac{k\nu}{(1+\nu)(1-2\nu)}$$

$\mathrm{Sym}\{\mathbf{A}\}$ is the symmetric component of matrix $\mathbf{A}$

The relation between the Piola stress $\mathbf{P}$ and $\mathbf{F}$ can be derived as follows:

$$\delta\boldsymbol{\epsilon} = \frac{1}{2}\left(\delta\mathbf{F} + \delta\mathbf{F}^T\right) = \mathrm{Sym}\{\delta\mathbf{F}\}$$

Due to the symmetry of $\boldsymbol{\epsilon}$ and $\mathbf{I}$

$$\boldsymbol{\epsilon}:\delta\boldsymbol{\epsilon} = \boldsymbol{\epsilon}:\mathrm{Sym}\{\delta\mathbf{F}\} = \boldsymbol{\epsilon}:\delta\mathbf{F} \qquad \mathrm{tr}(\delta\boldsymbol{\epsilon}) = \mathbf{I}:\mathrm{Sym}\{\delta\mathbf{F}\} = \mathbf{I}:\delta\mathbf{F}$$

$$\delta\Psi = 2\mu\boldsymbol{\epsilon}:\delta\boldsymbol{\epsilon} + \lambda\mathrm{tr}(\boldsymbol{\epsilon})\mathrm{tr}(\delta\boldsymbol{\epsilon}) = \underbrace{\left[2\mu\boldsymbol{\epsilon} + \lambda\mathrm{tr}(\boldsymbol{\epsilon})\mathbf{I}\right]}_{=\partial\Psi/\partial\mathbf{F}} : \delta\mathbf{F}$$

Since $\mathbf{P} = \frac{\partial\Psi}{\partial\mathbf{F}}$

$$\text{Thus} \quad \mathbf{P} = 2\mu\boldsymbol{\epsilon} + \lambda\mathrm{tr}(\boldsymbol{\epsilon})\mathbf{I}$$

or, after one final substitution for $\boldsymbol{\epsilon}$ (and a few algebraic reductions):

$$\mathbf{P}(\mathbf{F}) = \mu(\mathbf{F} + \mathbf{F}^T - 2\mathbf{I}) + \lambda\mathrm{tr}(\mathbf{F}-\mathbf{I})\mathbf{I}.$$

These expressions allow us to make the following observations:

- The stress $\mathbf{P}$ is a *linear* function of the deformation gradient. As we will see in chapter 4 this would also result on the nodal elastic forces having a linear dependence on nodal positions. As a consequence, this constitutive model is characterized by a significantly lower computational cost than other, nonlinear materials.
- Since the small strain tensor was designed to be accurate exclusively in a small deformation scenario, it would only be advisable to use linear elasticity when the magnitude of motion is small. For example, a rigid motion $\vec{\phi}(\vec{X}) = \mathbf{R}\vec{X} + \vec{t}$ would generally produce a non-zero strain $\epsilon = \frac{1}{2}(\mathbf{R} + \mathbf{R}^T) - \mathbf{I}$ and ultimately a nonzero stress, even though no shape change has taken place.

The Partial Differential Equation form of linear elasticity

For this simple material model it is relatively straightforward to derive the differential equation that defines an equilibrium configuration. Assume an externally applied force distribution $\vec{f}_{\text{ext}}(\vec{X})$. When the object has settled to an equilibrium (rest) configuration, the deformation function will satisfy:

$$\mathbf{divP} + \vec{f}_{\text{ext}} = 0 \Rightarrow \sum_{j=1}^{3} P_{ij,j} + f_{\text{ext}}^{(i)} = 0 \Rightarrow \qquad [\text{for } i = 1, 2, 3]$$

$$\Rightarrow -\sum_{j=1}^{3} \frac{\partial}{\partial X_j} \left[\mu(\phi_{i,j} + \phi_{j,i} - 2\delta_{ij}) + \delta_{i,j} \sum_{k=1}^{3} \lambda(\phi_{k,k} - 1) \right] = f_{\text{ext}}^{(i)} \Rightarrow$$

$$\Rightarrow -\sum_{j=1}^{3} \left[\mu(\phi_{i,jj} + \phi_{j,ij}) + \delta_{i,j} \sum_{k=1}^{3} \lambda \phi_{k,kj} \right] = f_{\text{ext}}^{(i)} \Rightarrow$$

$$\Rightarrow -\sum_{j=1}^{3} [\mu(\phi_{i,jj} + \phi_{j,ji})] - \sum_{k=1}^{3} \lambda \phi_{k,ki} = f_{\text{ext}}^{(i)} \Rightarrow \qquad \phi_{j,ij} = \phi_{j,ji}$$

$$\Rightarrow -\sum_{j=1}^{3} [\mu \phi_{i,jj} + (\mu + \lambda)\phi_{j,ji}] = f_{\text{ext}}^{(i)} \Rightarrow$$

Summation variables j and k are interchangable

$$\Rightarrow -\mu \Delta \phi_i - (\mu + \lambda) \frac{\partial}{\partial X_i} [\nabla \cdot \vec{\phi}] = f_{\text{ext}}^{(i)} \Rightarrow$$

$$\Rightarrow -\mu \Delta \vec{\phi} - (\mu + \lambda) \nabla [\nabla \cdot \vec{\phi}] = \vec{f}_{\text{ext}}$$

Which is a *linear*, second order Partial Differential Equation.

3.3 St. Venant-Kirchhoff model

With the understanding that the small strain tensor is a mere approximation of the rotationally invariant Green strain $\mathbf{E}$, it makes sense to attempt an improvement of the linear elasticity model by using $\mathbf{E}$ in the place of $\boldsymbol{\epsilon}$ in equation (3.2):

$$\Psi(\mathbf{F}) = \mu \mathbf{E} : \mathbf{E} + \frac{\lambda}{2} \mathrm{tr}^2(\mathbf{E})$$

The resulting constitutive model is called a *St. Venant-Kirchhoff material*, and is the first truly nonlinear material we will examine. The first Piola-Kirchhoff stress tensor can be computed via a process similar to the one followed for linear elasticity:

$$\delta \mathbf{E} = \frac{1}{2} \left(\delta \mathbf{F}^T \mathbf{F} + \mathbf{F}^T \delta \mathbf{F} \right) = \mathrm{Sym}\{ \mathbf{F}^T \delta \mathbf{F} \}$$

Due to the symmetry of $\mathbf{E}$ and $\mathbf{I}$

$$\mathbf{E} : \delta \mathbf{E} = \mathbf{E} : \left\{ \mathbf{F}^T \delta \mathbf{F} \right\} = \{ \mathbf{F} \mathbf{E} \} : \delta \mathbf{F} \qquad \mathrm{tr}(\delta \mathbf{E}) = \mathbf{I} : \left\{ \mathbf{F}^T \delta \mathbf{F} \right\} = \mathbf{F} : \delta \mathbf{F}$$

$$\delta \Psi = 2\mu \mathbf{E} : \delta \mathbf{E} + \lambda \mathrm{tr}(\mathbf{E}) \mathrm{tr}(\delta \mathbf{E}) = \underbrace{\mathbf{F} \left[2\mu \mathbf{E} + \lambda \mathrm{tr}(\mathbf{E}) \mathbf{I} \right]}_{= \partial \Psi / \partial \mathbf{F}} : \delta \mathbf{F}$$

$$\text{Thus} \quad \mathbf{P}(\mathbf{F}) = \mathbf{F} \left[2\mu \mathbf{E} + \lambda \mathrm{tr}(\mathbf{E}) \mathbf{I} \right]. \tag{3.3}$$

This is a rotationally invariant model; deformations that differ by a rigid body transformation are guaranteed to have the same strain energy. As a consequence a St. Venant-Kirchhoff material exhibits plausible material response in many large deformation scenarios where linear elasticity would not be applicable. Equation (3.3) indicates that stress is a 3rd degree polynomial function of the components of $\mathbf{F}$; after discretization, nodal forces will likewise be expressed as cubic polynomials of nodal positions.

Although the St. Venant-Kirchhoff model offers significant benefits over a linear elastic model, its scope is limited to a certain degree due to its poor resistance to forceful compression: as a St. Venant-Kirchhoff elastic body is compressed, starting from its undeformed configuration, it reacts with a restorative force which initially grows with the degree of compression. However, once a critical compression threshold is reached ($\approx 58\%$ of undeformed dimensions, when compression occurs along a single axis) the strength of the restorative force reaches a maximum. Further compression will be met with *decreasing* resistance, in fact the restorative force will vanish as the object is compressed all the way down to zero volume (an indication of this is that when $\mathbf{F} = \mathbf{0}$ we also have $\mathbf{P} = \mathbf{0}$). Continued compression past the point of zero volume (forcing the material to invert) will then create a restorative force that pushes the body towards complete inversion (reflection) along one or more axes. In practical computer simulation examples this behavior often manifests itself as a tendency of the material to locally tangle and invert itself when subjected to strong compressive forces or kinematic constraints.

3.4 Corotated linear elasticity

The use of the quadratic Green strain in the St. Venant-Kirchhoff guaranteed the rotational invariance of the constitutive model. At the same time, the increased complexity inherent in highly nonlinear materials leads to unintended side effects, such as the non-physical zero stress configurations of St. Venant-Kirchhoff materials under extreme compression. *Corotated linear elasticity* is a constitutive model that attempts to combine the simplicity of the stress-deformation relationship in a linear material with just enough nonlinear characteristics to secure rotational invariance.

Using the polar decomposition $\mathbf{F} = \mathbf{RS}$ we construct a new strain measure as $\boldsymbol{\epsilon}_{\mathrm{C}} = \mathbf{S} - \mathbf{I}$, which is linear on the symmetric tensor $\mathbf{S}$ obtained by factoring away the rotational component of $\mathbf{F}$. Replacing the small strain tensor in equation (3.2) we obtain the energy for corotational elasticity:

$$\Psi(\mathbf{F}) = \mu\boldsymbol{\epsilon}_{\mathrm{C}} : \boldsymbol{\epsilon}_{\mathrm{C}} + \frac{\lambda}{2}\mathrm{tr}^2(\boldsymbol{\epsilon}_{\mathrm{C}}) = \mu\|\mathbf{S} - \mathbf{I}\|_F^2 + (\lambda/2)\mathrm{tr}^2(\mathbf{S} - \mathbf{I})$$

which can also be equivalently written in any of the following ways:

$$\begin{aligned} \Psi(\mathbf{F}) &= \mu\|\mathbf{F} - \mathbf{R}\|_F^2 + (\lambda/2)\mathrm{tr}^2(\mathbf{R}^T\mathbf{F} - \mathbf{I}) \\ \Psi(\mathbf{F}) &= \mu\|\boldsymbol{\Sigma} - \mathbf{I}\|_F^2 + (\lambda/2)\mathrm{tr}^2(\boldsymbol{\Sigma} - \mathbf{I}) \end{aligned} \tag{3.4}$$

where $\boldsymbol{\Sigma}$ is the diagonal matrix with the singular values of $\mathbf{F}$, from the Singular Value Decomposition $\mathbf{F} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$. We can show that the 1st Piola-Kirchhoff stress tensor for corotated linear elasticity is given by:

$$\begin{aligned} \mathbf{P}(\mathbf{F}) &= \mathbf{R}\left[2\mu\boldsymbol{\epsilon}_{\mathrm{C}} + \lambda\mathrm{tr}(\boldsymbol{\epsilon}_{\mathrm{C}})\mathbf{I}\right] = \mathbf{R}\left[2\mu(\mathbf{S} - \mathbf{I}) + \lambda\mathrm{tr}(\mathbf{S} - \mathbf{I})\mathbf{I}\right] \\ &= 2\mu(\mathbf{F} - \mathbf{R}) + \lambda\mathrm{tr}(\mathbf{R}^T\mathbf{F} - \mathbf{I})\mathbf{R} \end{aligned} \tag{3.5}$$

Proof of the stress formula

Taking differentials of the Singular Value Decomposition $\mathbf{F} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$ we have:

$$\begin{aligned} \delta\mathbf{F} &= (\delta\mathbf{U})\boldsymbol{\Sigma}\mathbf{V}^T + \mathbf{U}(\delta\boldsymbol{\Sigma})\mathbf{V}^T + \mathbf{U}\boldsymbol{\Sigma}\delta\mathbf{V}^T \Rightarrow \\ \Rightarrow \mathbf{U}^T(\delta\mathbf{F})\mathbf{V} &= \underbrace{(\mathbf{U}^T\delta\mathbf{U})\boldsymbol{\Sigma}}_{(*)} + \delta\boldsymbol{\Sigma} + \underbrace{\boldsymbol{\Sigma}(\mathbf{V}^T\delta\mathbf{V})^T}_{(**)} \end{aligned} \tag{3.6}$$

For any orthogonal matrix $\mathbf{Q}$ we have

$$\mathbf{Q}^T\mathbf{Q} = \mathbf{I} \Rightarrow \delta(\mathbf{Q}^T\mathbf{Q}) = \mathbf{0} \Rightarrow (\delta\mathbf{Q})^T\mathbf{Q} + \mathbf{Q}^T\delta\mathbf{Q} = \mathbf{0} \Rightarrow (\mathbf{Q}^T\delta\mathbf{Q})^T = -\mathbf{Q}^T\delta\mathbf{Q}$$

Thus, the matrices marked with $(*)$ and $(**)$ above are column- and row-scaled versions of skew symmetric matrices, and consequently have zero diagonal elements.

This implies that if we restrict equation (3.6) to its diagonal component only, terms $(*)$ and $(**)$ will vanish to yield the final expression for the differential of $\mathbf{\Sigma}$:

$$\delta\mathbf{\Sigma} = \text{Diag}\{\mathbf{U}^T(\delta\mathbf{F})\mathbf{V}\}$$

Using this result, the differential of equation (3.4) becomes:

$$\begin{aligned}
\delta\Psi &= 2\mu(\mathbf{\Sigma}-\mathbf{I}):\delta\mathbf{\Sigma} + \lambda\text{tr}(\mathbf{\Sigma}-\mathbf{I})\text{tr}(\delta\mathbf{\Sigma}) \\
&= 2\mu(\mathbf{\Sigma}-\mathbf{I}):(\mathbf{U}^T\delta\mathbf{F}\mathbf{V}) + \lambda\text{tr}\left[\mathbf{V}(\mathbf{\Sigma}-\mathbf{I})\mathbf{V}^T\right]\text{tr}(\mathbf{U}^T\delta\mathbf{F}\mathbf{V}) \\
&= 2\mu\left[\mathbf{U}(\mathbf{\Sigma}-\mathbf{I})\mathbf{V}^T\right]:\delta\mathbf{F} + \lambda\text{tr}(\mathbf{S}-\mathbf{I})\text{tr}\left[(\mathbf{U}\mathbf{V}^T)^T\delta\mathbf{F}\right] \\
&= 2\mu(\mathbf{F}-\mathbf{R}):\delta\mathbf{F} + \lambda\text{tr}(\mathbf{S}-\mathbf{I})\mathbf{R}:\delta\mathbf{F} = \mathbf{P}:\delta\mathbf{F}
\end{aligned}$$

from which equation (3.5) follows.

The motivation behind corotational elasticity is to mimic what linear elasticity would have been, if the undeformed configuration had been rotated in the same way as encoded in the rotational factor $\mathbf{R}$ from the polar decomposition. Of course, in typical deformations where the value of $\mathbf{R}$ varies across the domain, making the transition from linear to corotated elasticity more complex than a change of variables due to a (constant) rotation of the undeformed configuration. From a computational cost perspective, the overhead of corotated vs. linear elasticity includes the cost of the polar decomposition, and the need to employ nonlinear solvers for certain types of simulation.

3.5 Isotropic materials and invariants

The constitutive models of St. Venant-Kirchoff and Corotated linear elasticity have been constructed to be rotationally invariant. We can formally define this property by considering a pair of deformations, denoted by their deformation maps $\vec{\phi}_1(\vec{X})$ and $\vec{\phi}_2(\vec{X})$, that differ only by a rigid body transform, specifically:

$$\vec{\phi}_2(\vec{X}) = \mathbf{R}\vec{\phi}_1(\vec{X}) + \vec{t}, \quad \text{where } \mathbf{R} \text{ is a } 3\times 3 \text{ rotation matrix.} \tag{3.7}$$

A constitutive model is rotationally invariant if and only if it guarantees that the strain energy will satisfy $E[\phi_1] = E[\phi_2]$ for any such deformation pair. For hyperelastic materials, an equivalent definition can be stated in terms of the strain energy density function. By taking gradients, we can see that any two deformations that satisfy equation (3.7) will have deformation gradients related as $\mathbf{F}_2 = \mathbf{R}\mathbf{F}_1$. The energy density associated with these deformations must satisfy $\Psi(\mathbf{F}_1) = \Psi(\mathbf{F}_2)$, leading to the following equivalent definition of rotational invariance:

Definition: A hyperelastic constitutive model is *rotationally invariant* if and only if the strain energy density satisfies

$$\Psi(\mathbf{RF}) = \Psi(\mathbf{F})$$

for any value of the deformation gradient $\mathbf{F}$ and any 3×3 rotation matrix $\mathbf{R}$.

A consequence of this definition is that the strain energy in rotationally invariant models can be expressed solely as a function of the symmetric factor $\mathbf{S}$ from the polar decomposition of $\mathbf{F} = \mathbf{RS}$, since:

$$\Psi(\mathbf{F}) = \Psi(\mathbf{RS}) = \Psi(\mathbf{S})$$

Although some model may be define Ψ directly as a function of $\mathbf{S}$ (corotated elasticity was presented this way), we may avoid the need to compute the polar decomposition, if we are able to express Ψ as a function of some other intermediate quantity, which is a function of $\mathbf{S}$, yet also computable without an explicit polar decomposition. For example, St. Venant-Kirchhoff materials defined the energy density as a function of the Green strain $\mathbf{E} = \frac{1}{2}(\mathbf{S}^2 - \mathbf{I})$, which although fully determined by $\mathbf{S}$ can also be computed without an explicit polar decomposition as $\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I})$.

A similar, yet distinct property of certain constitutive models (including St. Venant-Kirchhoff and Corotated linear elasticity) is that of *isotropy*. In plain terms, a material is isotropic if its resistance to deformation is the same along all possible orientations that such deformation may be applied. Rubber and metal would be examples of isotropic materials, as they do not exhibit any particular direction/orientation along which are softer or stiffer. Steel-reinforced concrete would be an example of an anisotropic material, as its resistance to deformation is notably different along the direction of the steel supports, compared to a direction perpendicular to them. Human muscles are also quoted as an anisotropic structure, as a distinct material response is observed along the direction aligned with muscle fibers.

Isotropy is a property that needs to be assessed on a local scale, as it is always possible to generate directional features in larger structures by arranging material in specific ways (think of suspension bridges built from otherwise isotropic steel). In terms of a quantitative criterion for isotropy, we can think of an infinitesimal *spherical* volume of material dV, and consider the strain energy resulting from a prescribed deformation. Now, consider the scenario where we first transform the sphere dV by *rotating it about its center* and then apply the same deformation. If the material is isotropic, both scenarios would lead to the same strain energy. This is concretely expressed using the strain energy function, as follows:

Definition: A hyperelastic constitutive model is *isotropic* if and only if the strain energy density satisfies

$$\Psi(\mathbf{FQ}) = \Psi(\mathbf{F})$$

for any value of the deformation gradient $\mathbf{F}$ and any 3×3 rotation matrix $\mathbf{Q}$. A material that is both rotationally invariant and isotropic would satisfy

$$\Psi(\mathbf{RFQ}) = \Psi(\mathbf{F})$$

for arbitrary rotations $\mathbf{R}$ and $\mathbf{Q}$.

Using the Singular Value Decomposition $\mathbf{F} = \mathbf{U\Sigma V}^T$ we conclude that rotationally invariant, isotropic materials satisfy:

$$\Psi(\mathbf{F}) = \Psi(\mathbf{U\Sigma V}^T) = \Psi(\mathbf{\Sigma}).$$

While the strain energy for rotationally invariant materials was a function only of 6 out of 9 degrees of freedom in $\mathbf{F}$ (those captured in the symmetric $\mathbf{S}$), for materials that are also isotropic the energy density is actually only a function of the three singular values of $\mathbf{F}$. Equation (3.4) reveals that this is certainly the case for corotated linear elasticity. St. Venant-Kirchhoff can also be shown to satisfy all criteria for isotropy, after some simple algebraic manipulations. An example of a material that is rotationally invariant but *not* isotropic is described by the energy:

$$\Psi(\mathbf{F}) = \frac{k}{2}\vec{w}^T\mathbf{F}^T\mathbf{F}\vec{w}$$

where $\vec{w}$ is a given constant vector. This material behaves like a zero-restlength spring along the direction $\vec{w}$, while it does not have any resistance to deformation along directions perpendicular to $\vec{w}$.

Although it is possible to define an isotropic material by a relation between Ψ and $\mathbf{\Sigma}$ (which encodes the only 3 relevant degrees of freedom in $\mathbf{F}$), this is not necessarily the preferred approach, since the overhead of an SVD computation would be necessary when evaluating any of these quantities. St. Venant-Kirchhoff materials avoided the need for an explicit polar decomposition, by using the Green strain E to convey (qualitatively) the same information as $\mathbf{S}$, while using a computationally inexpensive formula. For isotropic materials, the purpose is served by the three *isotropic invariants* of the deformation gradient, which are equally expressive as the singular values, but can be computed inexpensively. Invariants are denoted by I_1, I_2, I_3 (or $I_1(\mathbf{F})$, etc., to emphasize the dependence on $\mathbf{F}$) and defined as:

$$I_1(\mathbf{F}) = \mathrm{tr}(\mathbf{F}^T\mathbf{F}), \quad I_2(\mathbf{F}) = \mathrm{tr}\left[(\mathbf{F}^T\mathbf{F})^2\right], \quad I_3(\mathbf{F}) = \det(\mathbf{F}^T\mathbf{F}) = (\det\mathbf{F})^2$$

Their relation to Σ is revealed by replacing $\mathbf{F}$ with its SVD in the previous expressions, where (after extensive cancellation) we obtain:

$$I_1 = \mathrm{tr}(\mathbf{\Sigma}^2) = \sum_{i=1}^{3} \sigma_i^2, \quad I_2 = \mathrm{tr}(\mathbf{\Sigma}^4) = \sum_{i=1}^{3} \sigma_i^4, \quad I_3 = \det(\mathbf{\Sigma}^2) = \prod_{i=1}^{3} \sigma_i^2$$

Also of use are the *derivatives* of the invariants with respect to the $\mathbf{F}$:

$$\begin{aligned}
\delta I_1 = \delta[\mathrm{tr}(\mathbf{F}^T\mathbf{F})] = 2\mathrm{tr}(\mathbf{F}^T\delta\mathbf{F}) = (2\mathbf{F}) : \delta\mathbf{F} \quad &\Rightarrow \quad \frac{\partial I_1}{\partial \mathbf{F}} = 2\mathbf{F} \\
\delta I_2 = \delta[\mathrm{tr}(\mathbf{F}^T\mathbf{F}\mathbf{F}^T\mathbf{F})] = 4\mathrm{tr}(\mathbf{F}^T\mathbf{F}\mathbf{F}^T\delta\mathbf{F}) = (4\mathbf{F}\mathbf{F}^T\mathbf{F}) : \delta\mathbf{F} \quad &\Rightarrow \quad \frac{\partial I_2}{\partial \mathbf{F}} = 4\mathbf{F}\mathbf{F}^T\mathbf{F} \\
\delta I_3 = \delta[(\det \mathbf{F})^2] = 2 \det \mathbf{F} \cdot \delta[\det \mathbf{F}] = 2(\det \mathbf{F})^2 \mathbf{F}^{-T} : \delta\mathbf{F} \quad &\Rightarrow \quad \frac{\partial I_3}{\partial \mathbf{F}} = 2I_3\mathbf{F}^{-T}
\end{aligned}$$

When the common practice of defining an isotropic constitive model via invariants is followed, the strain energy density is provided as a function $\Psi(I_1, I_2, I_3)$. In such case, we can use the chain rule to compute the stress $\mathbf{P}$ as:

$$\mathbf{P} = \frac{\partial \Psi(I_1, I_2, I_3)}{\partial \mathbf{F}} = \frac{\partial \Psi}{\partial I_1}\frac{\partial I_1}{\partial \mathbf{F}} + \frac{\partial \Psi}{\partial I_2}\frac{\partial I_2}{\partial \mathbf{F}} + \frac{\partial \Psi}{\partial I_3}\frac{\partial I_3}{\partial \mathbf{F}}, \quad \text{or, after substitution:}$$

$$\boxed{\mathbf{P}(\mathbf{F}) = \frac{\partial \Psi}{\partial I_1} \cdot 2\mathbf{F} + \frac{\partial \Psi}{\partial I_2} \cdot 4\mathbf{F}\mathbf{F}^T\mathbf{F} + \frac{\partial \Psi}{\partial I_3} \cdot 2I_3\mathbf{F}^{-T}} \tag{3.8}$$

Finally, we note the additional invariant $J = \det \mathbf{F} = \sqrt{I_3}$ that is often used in replacement of I_3 while defining certain constitutive models. This quantity has an important physical interpretation as it represents the *fraction of volume change* due to deformation: a value of $J = 1$ implies that volume is preserved exactly while, $J = 2$ would indicate an expansion to twice the undeformed volume and $J = 0.2$ would be a compression down to 20% of the rest volume.

3.6 Neohookean elasticity

An example of an isotropic constitutive model defined via isotropic invariants is *Neohookean elasticity*:

$$\Psi(I_1, J) = \frac{\mu}{2}(I_1 - 3) - \mu \log(J) + \frac{\lambda}{2}\log^2(J), \quad \text{or equivalently}$$
$$\Psi(I_1, I_3) = \frac{\mu}{2}(I_1 - \log(I_3) - 3) + \frac{\lambda}{8}\log^2(I_3)$$

From this definition, we can easily compute

$$\frac{\partial \Psi}{\partial I_1} = \frac{\mu}{2} \quad \text{and} \quad \frac{\partial \Psi}{\partial I_3} = -\frac{\mu}{2I_3} + \frac{\lambda \log(I_3)}{4I_3}$$

Thus, using equation (3.8) we obtain:

$$\mathbf{P}(\mathbf{F}) = \mu\mathbf{F} - \mu\mathbf{F}^{-T} + \frac{\lambda \log(I_3)}{2}\mathbf{F}^{-T}$$
$$\text{or} \quad \mathbf{P}(\mathbf{F}) = \mu(\mathbf{F} - \mu\mathbf{F}^{-T}) + \lambda \log(J)\mathbf{F}^{-T}.$$

The Neohookean model has the following notable characteristics:

- By construction, the material exhibits a very strong reaction to extreme compression. Due to the logarithmic term $\log^2(J)$ in the energy, as $J \to 0$ we have $\Psi \to \infty$. This constructs a powerful energy barrier that strongly resists extreme compression. This is the only constitutive model we have seen so far that has this property; models discussed earlier in this chapter will allow the material to compress to zero volume, even invert, while only absorbing a finite amount of energy.

- Modeling materials as strongly incompressible amounts to using a very large value for the second Lamé coefficient (λ). Doing so in the case of Neohookean elasticity would emphasize the $\log^2(J)$ energy term, and strongly enforce $J = 1$ which produces an volume-preserving formulation. Incidentally, setting a high value for λ in the earlier constitutive models does not quite have the desired effect, as their respective terms scaled by λ do not correspond to true volume change (as J does). For example, a high λ value for linear elasticity would enforce

  $$\text{tr}(\mathbf{F} - \mathbf{I}) = 0 \Rightarrow \text{div}\left[\vec{\phi}(\vec{X}) - \vec{X}\right] = 0$$

  i.e. this will ensure that the displacement field $\vec{x}(\vec{X}) - \vec{X}$ is divergence free. This condition approximates volume preservation only for small deformations.

- The fact that the strain energy defines a (theoretically) impassable barrier at compression magnitudes leading to zero volume $J = 0$ implies that there is no mechanism for handling what happens when, accidentally, the simulated model is forced into a (theoretically impossible) inverted configuration. In such cases, energy and stress are undefined, since $J < 0$. We note that such inversions (although theoretically impossible) can easily occur in practice, as a result of nonphysical kinematic constraints, instability of time integration techniques, or inadequate convergence of numerical solvers. Should such a scenario arise, it is advised that the deformation gradient $\mathbf{F}$ be temporarily replaced by the nearest *physically plausible* value $\tilde{\mathbf{F}}$ (with $\det \tilde{\mathbf{F}} > \epsilon$).

Chapter 4

Discretization

The preceding chapters detailed a variety of physical laws that may be used to describe the response of elastic materials to deformation. Up to this point, these laws were expressed relative to a continuous deformation in space. Naturally, in order to enable numerical simulation all such laws have to be discretized; physical quantities such as the deformation map, the elastic strain energy, stress tensors and elastic forces all have to be reformulated as functions of our discrete state variables.

4.1 Energy and force discretization

When modeling a deformable body on the computer we only store the values of the deformation map $\phi(\vec{X})$ on a finite number of points $\vec{X}_1, \vec{X}_2, \ldots, \vec{X}_N$, corresponding to the vertices of a discretization mesh. The respective deformed vertex locations $\vec{x}_i = \phi(\vec{X}_i),\ i = 1, 2, \ldots, N$ are our discrete degrees of freedom, and we can write $\mathbf{x} = (\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N)$ for the aggregate state of our model. As a first step, we need to specify a method for reconstructing a continuous deformation map $\hat{\phi}$ from the discrete samples $\vec{x}_i = \phi(\vec{X}_i)$. In essence this is just a choice of an interpolation scheme. For example, if a tetrahedral mesh is used to describe the deforming body, barycentric interpolation will extend the nodal deformations to the entire interior of the mesh. Trilinear interpolation would be a natural choice for lattice discretizations. At any rate, we denote the interpolated deformation map by $\hat{\phi}(\vec{X}; \mathbf{x})$ which emphasizes that this interpolated deformation is dependent on the discrete state $\mathbf{x}$.

For a hyperelastic material, the strain energy of any given deformation $\phi(\vec{x})$ is computed by integrating the energy density Ψ over the entire body Ω:

$$E[\phi] := \int_\Omega \Psi(\mathbf{F}) d\vec{X}$$

We can now define a discrete energy, expressed as a function of the degrees of freedom $\mathbf{x}$, by simply plugging the interpolated deformation $\hat{\phi}$ into the definition of

the strain energy

$$E(\mathbf{x}) := E\left[\hat{\phi}(\vec{X};\mathbf{x})\right] = \int_{\Omega} \Psi\left(\hat{\mathbf{F}}(\vec{X};\mathbf{x})\right) d\vec{X} \tag{4.1}$$

where $\hat{\mathbf{F}}(\vec{X};\mathbf{x}) := \partial\hat{\phi}(\vec{X};\mathbf{x})/\partial\vec{X}$ is the deformation gradient computed from the interpolated map $\hat{\phi}$. It is understandable that equation (4.1) may appear quite cryptic at this point, since both the energy $\Psi(\mathbf{F})$ and the interpolated $\hat{\phi}$ are likely defined via complex formulas. In this chapter we will focus on two common spatial discretizations (tetrahedral meshes and Cartesian hexahedral lattices) and explain how the energy in equation (4.1) and all its derived quantities can be evaluated systematically and efficiently.

Having defined the discrete energy $E(\mathbf{x})$ we can now compute the elastic forces associated with individual mesh nodes, by taking the negative gradient of the elastic energy with respect to the corresponding degree of freedom:

$$\vec{f}_i(\mathbf{x}) = -\frac{\partial E(\mathbf{x})}{\partial \vec{x}_i} \quad \text{or, collectively} \quad \mathbf{f} := (\vec{f}_1, \vec{f}_2, \ldots, \vec{f}_N) = -\frac{\partial E(\mathbf{x})}{\partial \mathbf{x}}$$

Outline of a brief (albeit over-simplified) "proof" ...

For simplicity, let us assume that (a) the deforming body is not subject to any internal friction forces which would reduce its overall energy, and (b) the mass of the body is distributed exclusively to the mesh nodes. The total energy of the body is the sum of strain energy (E) and kinetic energy (K) as follows:

$$E_{\text{total}} = E(\mathbf{x}) + K(\mathbf{v}) = E(\mathbf{x}) + \sum_{i=1}^{N} \frac{1}{2} m_i \|\vec{v}_i\|^2$$

Since no friction forces are in effect the total energy is conserved over time, thus:

$$\frac{\partial}{\partial t} E_{\text{total}} = 0 \Rightarrow \sum_{i=1}^{N} \left[\frac{\partial E(\mathbf{x})}{\partial \vec{x}_i} \cdot \vec{v}_i + m_i \vec{a}_i \cdot \vec{v}_i \right] = 0$$

Since the last equality holds for any value of the velocities $\{\vec{v}_i\}$, we must have:

$$\frac{\partial E(\mathbf{x})}{\partial \vec{x}_i} + m_i \vec{a}_i = 0 \Rightarrow \vec{f}_i = m_i \vec{a}_i = -\frac{\partial E(\mathbf{x})}{\partial \vec{x}_i} \quad \text{for all} \quad i = 1, 2, \ldots, N$$

In practice, prior to computing each force, we first separate the energy integral of equation (4.1) into the contributions of individual elements Ω_e (e.g. triangles,

hexahedra, etc.) as follows:

$$E(\mathbf{x}) = \sum_e E^e(\mathbf{x}) = \sum_e \int_{\Omega_e} \Psi\left(\hat{\mathbf{F}}(\vec{X};\mathbf{x})\right) d\vec{X}$$

Subsequently, the force $\vec{f_i}$ on each node can be computed by adding the contributions of all elements in its immediate neighborhood $\mathcal{N}_i$:

$$\vec{f_i}(\mathbf{x}) = \sum_{e\in\mathcal{N}_i} \vec{f_i^e}(\mathbf{x}), \quad \text{where} \quad \vec{f_i^e}(\mathbf{x}) = -\frac{\partial E^e(\mathbf{x})}{\partial \vec{x}_i}$$

For simplicity, the following sections will focus on computing the nodal forces on an element-by-element basis, with the understanding that the aggregate forces are computed by accumulating the contributions from all elements in the mesh.

4.2 Linear tetrahedral elements

Tetrahedral meshes are among the most popular discrete volumetric geometry representations. At the same time, they offer one of the most straightforward options for constructing a discretization of the elasticity equations. The convenience of tetrahedral discretizations is largely due to the simple interpolation method they imply; the reconstructed deformation map $\hat{\phi}$ can be defined to be a *piecewise linear* function over each tetrahedron. Specifically, in every tetrahedron $\mathcal{T}_i$ we have

$$\hat{\phi}(\vec{X}) = \mathbf{A}_i\vec{X} + \vec{b}_i \quad \text{for all} \quad \vec{X} \in \mathcal{T}_i \tag{4.2}$$

where the matrix $\mathbf{A}_i \in \mathbf{R}^{3\times3}$ and the vector $\vec{b}_i \in \mathbf{R}^3$ are specific to each tetrahedron. The interpolation scheme implied by equation (4.2) is no other than simple barycentric interpolation on every element. Differentiating (4.2) with respect to $\vec{X}$ reveals that the deformation gradient $\mathbf{F} = \partial\hat{\phi}/\partial\vec{X} = \mathbf{A}_i$ is constant on each element, and as a consequence so will be any discrete strain measure and stress tensor; this justifies why linear tetrahedral elements are also referred to as *constant strain tetrahedra*.

For simplicity of notation we write

$$\phi(\vec{X}) = \mathbf{F}\vec{X} + \vec{b}$$

where we dropped the tetrahedron index, and replaced matrix $\mathbf{A}_i$ with its equal deformation gradient. Interestingly, it is possible to determine $\mathbf{F}$ (and $\vec{b}$, if desired) directly from the locations of the tetrahedron vertices, without involving any reasoning related to barycentric interpolation. Let us denote with $\vec{X}_1, \ldots, \vec{X}_4$ the undeformed (reference) locations of the tetrahedron vertices, and let $\vec{x}_1, \ldots, \vec{x}_4$

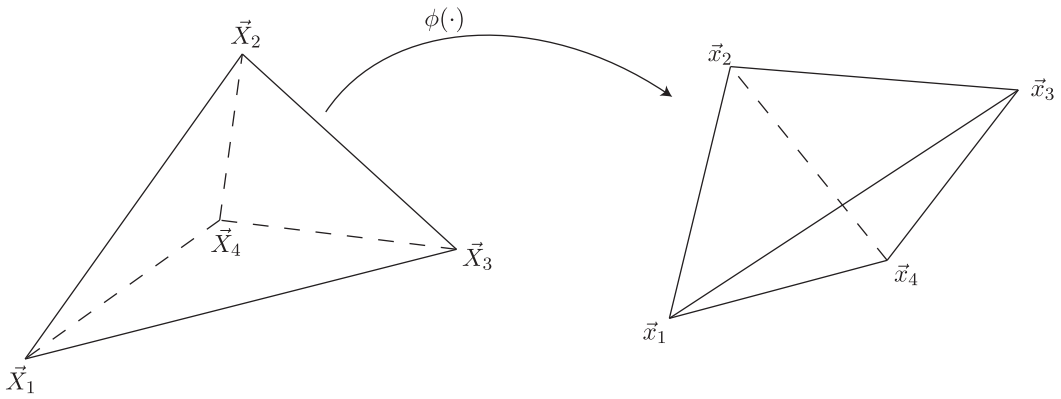

Figure 4.1: Reference (left) and deformed (right) shape of a linear tetrahedron

symbolize the respective deformed vertex locations as illustrated in figure 4.1. Each vertex must satisfy $\vec{x}_i = \phi(\vec{X}_i)$, or

$$\left\{ \begin{array}{l} \vec{x}_1 = \mathbf{F}\vec{X}_1 + \vec{b} \\ \vec{x}_2 = \mathbf{F}\vec{X}_2 + \vec{b} \\ \vec{x}_3 = \mathbf{F}\vec{X}_3 + \vec{b} \\ \vec{x}_4 = \mathbf{F}\vec{X}_4 + \vec{b} \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} \vec{x}_1 - \vec{x}_4 = \mathbf{F}\left(\vec{X}_1 - \vec{X}_4\right) \\ \vec{x}_2 - \vec{x}_4 = \mathbf{F}\left(\vec{X}_2 - \vec{X}_4\right) \\ \vec{x}_3 - \vec{x}_4 = \mathbf{F}\left(\vec{X}_3 - \vec{X}_4\right) \end{array} \right\}$$

where the last system was derived by subtracting the equation $\vec{x}_4 = \mathbf{F}\vec{X}_4 + \vec{b}$ from the three others, to eliminate the vector $\vec{b}$. It is possible to group the last three (vector) equations as a single matrix equation, by placing each one into the respective column of a 3×3 matrix:

$$\begin{aligned} \left[\begin{array}{ccc} \vec{x}_1 - \vec{x}_4 & \vec{x}_2 - \vec{x}_4 & \vec{x}_3 - \vec{x}_4 \end{array} \right] &= \left[\begin{array}{ccc} \mathbf{F}\left(\vec{X}_1 - \vec{X}_4\right) & \mathbf{F}\left(\vec{X}_2 - \vec{X}_4\right) & \mathbf{F}\left(\vec{X}_3 - \vec{X}_4\right) \end{array} \right] \\ \left[\begin{array}{ccc} \vec{x}_1 - \vec{x}_4 & \vec{x}_2 - \vec{x}_4 & \vec{x}_3 - \vec{x}_4 \end{array} \right] &= \mathbf{F}\left[\begin{array}{ccc} \vec{X}_1 - \vec{X}_4 & \vec{X}_2 - \vec{X}_4 & \vec{X}_3 - \vec{X}_4 \end{array} \right] \\ \mathbf{D}_s &= \mathbf{F}\mathbf{D}_m \end{aligned} \tag{4.3}$$

where

$$\mathbf{D}_s := \left[\begin{array}{ccc} x_1 - x_4 & x_2 - x_4 & x_3 - x_4 \\ y_1 - y_4 & y_2 - y_4 & y_3 - y_4 \\ z_1 - z_4 & z_2 - z_4 & z_3 - z_4 \end{array} \right] \tag{4.4}$$

is the *deformed shape matrix* and

$$\mathbf{D}_m := \left[\begin{array}{ccc} X_1 - X_4 & X_2 - X_4 & X_3 - X_4 \\ Y_1 - Y_4 & Y_2 - Y_4 & Y_3 - Y_4 \\ Z_1 - Z_4 & Z_2 - Z_4 & Z_3 - Z_4 \end{array} \right]$$

is called the *reference shape matrix* (or "material-space" shape matrix).

We note that $\mathbf{D}_m$ is a constant matrix, as it only depends on the vertex coordinates in the reference (undeformed) configuration; Furthermore, the undeformed volume of the tetrahedron equals $W = \frac{1}{6}|\det \mathbf{D}_m|$; assuming that the reference shape of the tetrahedron is non-degenerate (i.e. nonzero volume, $W \neq 0$), the matrix $\mathbf{D}_m$ is nonsingular and equation (4.3) can be solved for $\mathbf{F}$ as:

$$\mathbf{F} = \mathbf{D}_s \mathbf{D}_m^{-1} \quad \text{or} \quad \mathbf{F}(\mathbf{x}) = \mathbf{D}_s(\mathbf{x}) \mathbf{D}_m^{-1} \tag{4.5}$$

where the last expression emphasizes that the deformed degrees of freedom appear only in the expression for $\mathbf{D}_s$; while the constant $\mathbf{D}_m^{-1}$ is precomputed and stored.

Since $\mathbf{F}$ is constant over the linear tetrahedron, the strain energy of this element reduces to:

$$E_i = \int_{T_i} \Psi(\mathbf{F}) d\vec{X} = \Psi(\mathbf{F}_i) \int_{T_i} d\vec{X} = W \cdot \Psi(\mathbf{F}_i) \quad \text{or} \quad E(\mathbf{x}) = W \cdot \Psi(\mathbf{F}(\mathbf{x})) \tag{4.6}$$

We may subsequently use Equation (4.6) to derive the contribution of element $\mathcal{T}_i$ to the elastic forces on its four vertices as $\vec{f}_k^i = -\partial E_i(\mathbf{x}) / \partial \vec{x}_k$. In fact, the forces on all four vertices can be collectively computed via the following equations:

$$\mathbf{H} = \begin{bmatrix} \vec{f}_1 & \vec{f}_2 & \vec{f}_3 \end{bmatrix} = -W \mathbf{P}(\mathbf{F}) \mathbf{D}_m^{-T} \quad \text{and} \quad \vec{f}_4 = -\vec{f}_1 - \vec{f}_2 - \vec{f}_3 \tag{4.7}$$

$\mathbf{P}(\mathbf{F})$ is the Piola stress defined in section 2.4

Proof

Define $x_i^{(1)}, x_i^{(2)}, x_i^{(3)}$ to be the x-, y- and z- coordinates of the vertex $\vec{x}_i$. Likewise for the components of the nodal force $\vec{f}_i = (f_i^{(1)}, f_i^{(2)}, f_i^{(3)})$

Lemma For $i = 1, 2, 3$

$$\partial \mathbf{F} / \partial x_i^{(j)} = \mathbf{e}_j \mathbf{e}_i^T \mathbf{D}_m^{-1}$$

Proof From equation (4.3) we have $\partial \mathbf{D}_s / \partial x_i^{(j)} = \mathbf{e}_j \mathbf{e}_i^T$. The Lemma follows directly from this equation and $\mathbf{F} = \mathbf{D}_s \mathbf{D}_m^{-1}$.

We proceed to compute the force component:

$$H_{ji} = f_i^{(j)} = -\frac{\partial E(\mathbf{x})}{\partial x_i^{(j)}} = -W \frac{\partial \Psi(\mathbf{x})}{\partial \mathbf{F}} : \frac{\partial \mathbf{F}}{\partial x_i^{(j)}} = -W \mathbf{P}(\mathbf{F}) : \left(\mathbf{e}_j \mathbf{e}_i^T \mathbf{D}_m^{-1} \right) =$$

$$= -W \operatorname{tr} \left[\mathbf{P}(\mathbf{F}) \mathbf{D}_m^{-T} \mathbf{e}_i \mathbf{e}_j^T \right] = -W \mathbf{e}_j^T \mathbf{P}(\mathbf{F}) \mathbf{D}_m^{-T} \mathbf{e}_i = \left[-W \mathbf{P}(\mathbf{F}) \mathbf{D}_m^{-T} \right]_{ji}$$

Thus $\mathbf{H} = -W \mathbf{P}(\mathbf{F}) \mathbf{D}_m^{-T}$. The equation $\vec{f}_4 = -\vec{f}_1 - \vec{f}_2 - \vec{f}_3$ can be proved in a directly similar fashion, but is also a consequence of conservation of momentum; if the sum of all four nodal forces (which are internal to the body) did not sum to zero, this would violate conservation of linear momentum.

The computation of all elastic forces in a tetrahedral mesh is summarized in pseudocode as follows:

Algorithm 1 Batch computation of elastic forces on a tetrahedral mesh

procedure PRECOMPUTATION($\mathbf{x}, \mathbf{B}_m[1 \dots M], W[1 \dots M]$)
  for each $\mathcal{T}_e = (i, j, k, l) \in \mathcal{M}$ **do** ▷ M is the number of tetrahedra
    $\mathbf{D}_m \leftarrow \begin{bmatrix} X_i - X_l & X_j - X_l & X_k - X_l \\ Y_i - Y_l & Y_j - Y_l & Y_k - Y_l \\ Z_i - Z_l & Z_j - Z_l & Z_k - Z_l \end{bmatrix}$
    $\mathbf{B}_m[e] \leftarrow \mathbf{D}_m^{-1}$
    $W[e] \leftarrow \frac{1}{6} \det(\mathbf{D}_m)$ ▷ W is the undeformed volume of $\mathcal{T}_e$
  end for
end procedure
procedure COMPUTEELASTICFORCES($\mathbf{x}, \mathbf{f}, \mathcal{M}, \mathbf{B}_m[], W[]$)
  $\mathbf{f} \leftarrow \mathbf{0}$ ▷ $\mathcal{M}$ is a tetrahedral mesh
  for each $\mathcal{T}_e = (i, j, k, l) \in \mathcal{M}$ **do**
    $\mathbf{D}_s \leftarrow \begin{bmatrix} x_i - x_l & x_j - x_l & x_k - x_l \\ y_i - y_l & y_j - y_l & y_k - y_l \\ z_i - z_l & z_j - z_l & z_k - z_l \end{bmatrix}$
    $\mathbf{F} \leftarrow \mathbf{D}_s \mathbf{B}_m[e]$
    $\mathbf{P} \leftarrow \mathbf{P}(\mathbf{F})$ ▷ From the constitutive law
    $\mathbf{H} \leftarrow -W[e]\mathbf{P}\,(\mathbf{B}_m[e])^T$
    $\vec{f_i}$ += $\vec{h}_1$, $\vec{f_j}$ += $\vec{h}_2$, $\vec{f_k}$ += $\vec{h}_3$ ▷ $\mathbf{H} = \begin{bmatrix} \vec{h}_1 & \vec{h}_2 & \vec{h}_3 \end{bmatrix}$
    $\vec{f_l}$ += $(-\vec{h}_1 - \vec{h}_2 - \vec{h}_3)$
  end for
end procedure

4.3 Force differentials

We have seen how discrete nodal forces ($\mathbf{f}$) can be computed for an arbitrary constitutive model, given nodal positions ($\mathbf{x}$) as input. This is all that is necessary to implement an explicit (e.g. Forward Euler) time integration scheme; however implicit methods such as Backward Euler will also require a process for computing *force differentials*, i.e. linearized nodal force increments around a configuration $\mathbf{x}_*$, relative to a small nodal force displacement $\delta\mathbf{x}$. We denote this by:

$$\delta\mathbf{f} = \delta\mathbf{f}(\mathbf{x}_*; \delta\mathbf{x}) := \left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}_*} \cdot \delta\mathbf{x}$$

Although in this expression we used the *stiffness matrix* $\partial\mathbf{f}/\partial\mathbf{x}$ to aid in the definition of the force differential, in practice it may be preferable to avoid constructing

this matrix explicitly, as the construction cost and memory footprint associated with it may impact performance. Instead, we aim to compute the force differentials $\delta\mathbf{f}$ directly, using only the information in the current state $\mathbf{x}_*$, the displacement $\delta\mathbf{x}$ and a small amount of additional meta-data.

As was the case with force computation, we evaluate the force differential vector $\delta\mathbf{f} = (\delta\vec{f}_1, \delta\vec{f}_2, \ldots, \delta\vec{f}_N)$ on an element-by-element basis, accumulating the contribution of each element to the aggregate value of each of its nodes. Consequently, we only focus on the process for computing differentials of nodal forces for a single tetrahedron. As before, we can pack the differentials of the first three vertices ($\delta\vec{f}_1, \delta\vec{f}_2$ and $\delta\vec{f}_3$) in a single matrix representation:

$$\delta\mathbf{H} = \begin{bmatrix} \delta\vec{f}_1 & \delta\vec{f}_2 & \delta\vec{f}_3 \end{bmatrix}$$

Once $\delta\mathbf{H}$ has been evaluated, the force differential for the fourth node can be computed as $\delta\vec{f}_4 = -\delta\vec{f}_1 - \delta\vec{f}_2 - \delta\vec{f}_3$. Taking differentials on equation (4.7) we obtain the following expression for $\delta\mathbf{H}$:

$$\delta\mathbf{H} = -W\delta\mathbf{P}(\mathbf{F}; \delta\mathbf{F})\mathbf{D}_m^{-T}$$

Thus, the computation of nodal force differentials has been reduced to a computation of the stress differential $\delta\mathbf{F}$. There are two steps in completing this evaluation: (a) we need to construct the deformation gradient increment $\delta\mathbf{F}$ (the deformation gradient $\mathbf{F}$ itself is computed as detailed in the previous section) and (b) we need to provide a usable formula for $\delta\mathbf{P}(\mathbf{F}; \delta\mathbf{F})$.

We start with the differential of the deformation gradient $\delta\mathbf{F}$, which is easily computed by taking the differentials on equation (4.5) to obtain:

$$\delta\mathbf{F} = (\delta\mathbf{D}_s)\mathbf{D}_m^{-1}$$

Matrix $\delta\mathbf{D}_s$ itself is simply computed by arranging the nodal displacements in the same fashion as nodal positions were for $\mathbf{D}_s$:

$$\delta\mathbf{D}_s := \begin{bmatrix} \delta x_1 - \delta x_4 & \delta x_2 - \delta x_4 & \delta x_3 - \delta x_4 \\ \delta y_1 - \delta y_4 & \delta y_2 - \delta y_4 & \delta y_3 - \delta y_4 \\ \delta z_1 - \delta z_4 & \delta z_2 - \delta z_4 & \delta z_3 - \delta z_4 \end{bmatrix}$$

The one remaining task is to provide a concise formula for $\delta\mathbf{P}(\mathbf{F}; \delta\mathbf{F})$. By necessity, this will be a process that depends on the constitutive model itself. Here, we provide examples of this derivation for the St. Venant-Kirchhoff, and Neohookean material models:

Stress differentials for St. Venant-Kirchhoff materials

We start by assessing the differential of the Green strain tensor:

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I}) \Rightarrow \delta\mathbf{E} = \frac{1}{2}(\delta\mathbf{F}^T\mathbf{F} + \mathbf{F}^T\delta\mathbf{F})$$

We then proceed to compute the differential of the stress tensor itself:

$$\mathbf{P}(\mathbf{F}) = \mathbf{F}\left[2\mu\mathbf{E} + \lambda\mathrm{tr}(\mathbf{E})\mathbf{I}\right] \Rightarrow$$
$$\delta\mathbf{P}(\mathbf{F};\delta\mathbf{F}) = \delta\mathbf{F}\left[2\mu\mathbf{E} + \lambda\mathrm{tr}(\mathbf{E})\mathbf{I}\right] + \mathbf{F}\left[2\mu\delta\mathbf{E} + \lambda\mathrm{tr}(\delta\mathbf{E})\mathbf{I}\right]$$

Stress differentials for Neohookean materials

We will use without proof the following two expressions for the differential of the matrix inverse and matrix determinant:

$$\delta[\mathbf{F}^{-1}] = -\mathbf{F}^{-1}\delta\mathbf{F}\mathbf{F}^{-1}, \quad \text{also} \quad \delta[\mathbf{F}^{-T}] = -\mathbf{F}^{-T}\delta\mathbf{F}^T\mathbf{F}^{-T}$$
$$\delta[\det\mathbf{F}] = \det\mathbf{F}\cdot\mathrm{tr}(\mathbf{F}^{-1}\delta\mathbf{F})$$

With these results, the differential of $\mathbf{P}$ is computed as

$$\mathbf{P}(\mathbf{F}) = \mu(\mathbf{F} - \mathbf{F}^{-T}) + \lambda\log(J)\mathbf{F}^{-T} \Rightarrow$$
$$\Rightarrow \delta\mathbf{P}(\mathbf{F};\delta\mathbf{F}) = \mu(\delta\mathbf{F} + \mathbf{F}^{-T}\delta\mathbf{F}^T\mathbf{F}^{-T}) + \lambda\frac{\delta[\det\mathbf{F}]}{\mathbf{J}}\mathbf{F}^{-T} - \lambda\log(J)\mathbf{F}^T\delta\mathbf{F}^T\mathbf{F}^{-T}$$
$$\Rightarrow \delta\mathbf{P}(\mathbf{F};\delta\mathbf{F}) = \mu\delta\mathbf{F} + \left[\mu - \lambda\log(J)\right]\mathbf{F}^{-T}\delta\mathbf{F}^T\mathbf{F}^{-T} + \lambda\mathrm{tr}(\mathbf{F}^{-1}\delta\mathbf{F})\mathbf{F}^{-T}$$

The force differential computation is summarized in pseudocode as Algorithm (2).

4.4 An implicit time integration scheme

We are now in a position to describe a complete, implicit-time integration scheme for nonlinear elastic bodies. The formulation that follows is based on the Backward Euler method, and thus is unconditionally stable for any timestep Δt (subject to the nonlinear equations involved being solved to satisfactory accuracy). We will first introduce some notation:

- $\mathbf{f}_e(\mathbf{x}^*)$: Elastic forces at configuration $\mathbf{x}^*$, as defined in previous sections.

Algorithm 2 Batch computation of elastic force differential on a tetrahedral mesh. Assumes that the precomputation routine from algorithm 1 is also available.

1: **procedure** ComputeForceDifferentials($\mathbf{x}, \mathbf{f}, \delta\mathbf{x}, \delta\mathbf{f}, \mathcal{M}, \mathbf{B}_m[], W[]$)
2: $\quad\mathbf{f} \leftarrow \mathbf{0}$ ▷ $\mathcal{M}$ is a tetrahedral mesh
3: $\quad$**for each** $\mathcal{T}_e = (i, j, k, l) \in \mathcal{M}$ **do**
4: $\quad\quad\mathbf{D}_s \leftarrow \begin{bmatrix} x_i - x_l & x_j - x_l & x_k - x_l \\ y_i - y_l & y_j - y_l & y_k - y_l \\ z_i - z_l & z_j - z_l & z_k - z_l \end{bmatrix}$
5: $\quad\quad\delta\mathbf{D}_s \leftarrow \begin{bmatrix} \delta x_i - \delta x_l & \delta x_j - \delta x_l & \delta x_k - \delta x_l \\ \delta y_i - \delta y_l & \delta y_j - \delta y_l & \delta y_k - \delta y_l \\ \delta z_i - \delta z_l & \delta z_j - \delta z_l & \delta z_k - \delta z_l \end{bmatrix}$
6: $\quad\quad\mathbf{F} \leftarrow \mathbf{D}_s\mathbf{B}_m[e]$
7: $\quad\quad\delta\mathbf{F} \leftarrow (\delta\mathbf{D}_s)\mathbf{B}_m[e]$
8: $\quad\quad\delta\mathbf{P} \leftarrow \delta\mathbf{P}(\mathbf{F}; \delta\mathbf{F})$ ▷ From the stress derivative formula
9: $\quad\quad\delta\mathbf{H} \leftarrow -W[e](\delta\mathbf{P})\,(\mathbf{B}_m[e])^T$
10: $\quad\quad\delta\vec{f}_i \mathrel{+}= \delta\vec{h}_1,\ \delta\vec{f}_j \mathrel{+}= \delta\vec{h}_2,\ \delta\vec{f}_k \mathrel{+}= \delta\vec{h}_3$ ▷ $\delta\mathbf{H} = \left[\delta\vec{h}_1\ \delta\vec{h}_2\ \delta\vec{h}_3\right]$
11: $\quad\quad\delta\vec{f}_l \mathrel{+}= (-\delta\vec{h}_1 - \delta\vec{h}_2 - \delta\vec{h}_3)$
12: $\quad$**end for**
13: **end procedure**

- $\mathbf{K}(\mathbf{x}^*) = -\left.\frac{\partial \mathbf{f}_e}{\partial \mathbf{x}}\right|_{\mathbf{x}^*}$: This is the elasticity stiffness matrix evaluated around the configuration $\mathbf{x}^*$. In most cases, the matrix $\mathbf{K}$ will never be explicitly constructed; interative solvers that involve this matrix will only require the evaluation of matrix-vector products of the form $\mathbf{Kw}$. These products can be computed in a matrix-free fashion by calling the force differential computation procedure detailed in Algorithm (2) with an argument $\delta\mathbf{x} \leftarrow (-\mathbf{w})$

- $\mathbf{f}_d(\mathbf{x}^*, \mathbf{v}^*) = -\gamma\mathbf{K}(\mathbf{x}^*)\mathbf{v}^*$: Damping forces at position $\mathbf{x}^*$ and velocity $\mathbf{v}^*$ according to the Rayleigh damping model. The parameter γ does not have a predetermined range (it is not confined to an interval such as $[0, 1]$) and can be spatially varying, or constant for simplicity.

- $\mathbf{f}(\mathbf{x}^*, \mathbf{v}^*) = \mathbf{f}_e(\mathbf{x}^*) + \mathbf{f}_d(\mathbf{x}^*, \mathbf{v}^*)$: The aggregate forces, including elastic and damping components.

- $\mathbf{M}$: The mass matrix. We shall assume $\mathbf{M}$ is lumped to diagonal form.

In order to define a backward Euler integration scheme, we will need to maintain both the position ($\mathbf{x}^n$) and the velocity ($\mathbf{v}^n$) of the deforming body at time t^n. Alternatively, it would have been possible to maintain just the two previous positions $\mathbf{x}^n$ and $\mathbf{x}^{n-1}$. The Backward Euler scheme computes the positions $\mathbf{x}^{n+1}$ and

velocities $\mathbf{v}^{n+1}$ at time $t^{n+1}(:= t^n + \Delta t)$ as the solution of the (nonlinear) system of equations:

$$\begin{aligned} \mathbf{x}^{n+1} &= \mathbf{x}^n + \Delta t \mathbf{v}^{n+1} && (4.8) \\ \mathbf{v}^{n+1} &= \mathbf{v}^n + \Delta t \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}^{n+1}, \mathbf{v}^{n+1}) \\ &= \mathbf{v}^n + \Delta t \mathbf{M}^{-1} \Big(\mathbf{f}_e(\mathbf{x}^{n+1}) + \mathbf{f}_d(\mathbf{x}^{n+1}, \mathbf{v}^{n+1}) \Big) && (4.9) \end{aligned}$$

Since the Backward Euler system is nonlinear due to equation (4.9), we shall define an iterative process to compute the unknowns $\mathbf{x}^{n+1}$ and $\mathbf{v}^{n+1}$. We will construct sequences of approximations $\mathbf{x}^{n+1}_{(0)}, \mathbf{x}^{n+1}_{(1)}, \mathbf{x}^{n+1}_{(2)}, \ldots$ and $\mathbf{v}^{n+1}_{(0)}, \mathbf{v}^{n+1}_{(1)}, \mathbf{v}^{n+1}_{(2)}, \ldots$ respectively, such that $\mathbf{x}^{n+1}_{(k)} \overset{k\to\infty}{\longrightarrow} \mathbf{x}^{n+1}$ and $\mathbf{v}^{n+1}_{(k)} \overset{k\to\infty}{\longrightarrow} \mathbf{v}^{n+1}$ respectively. We will use the positions and velocities at the previous time step as initial guesses, i.e. $\mathbf{x}^{n+1}_{(0)} = \mathbf{x}^n, \mathbf{v}^{n+1}_{(0)} = \mathbf{v}^n$.

We introduce the position and velocity *correction* variables, defined as

$$\Delta \mathbf{x}_{(k)} := \mathbf{x}^{n+1}_{(k+1)} - \mathbf{x}^{n+1}_{(k)} \quad \text{and} \quad \Delta \mathbf{v}_{(k)} := \mathbf{v}^{n+1}_{(k+1)} - \mathbf{v}^{n+1}_{(k)}.$$

In most cases, unless there is risk of ambiguity, we will drop the subscript and denote these corrections simply as $\Delta \mathbf{x}, \Delta \mathbf{v}$. At every step of our iterative scheme for the nonlinear Backward Euler system, we will linearize equations (4.8) and (4.9) around the current iterate $\mathbf{x}^{n+1}_{(k)}, \mathbf{v}^{n+1}_{(k)}$, and the solution of the linearized system will define the next iterate $\mathbf{x}^{n+1}_{(k+1)}, \mathbf{v}^{n+1}_{(k+1)}$.

Lemma 1. $\Delta \mathbf{x} = \Delta t \Delta \mathbf{v}$.

Proof. Equation (4.8) is in fact linear. Therefore, at every iteration it will simply linearize to itself, i.e.

$$\mathbf{x}^{n+1}_{(k)} = \mathbf{x}^n + \Delta t \mathbf{v}^{n+1}_{(k)}, \quad \text{for all } k.$$

Subtracting the above equations for iterations k and $k+1$, we obtain

$$\mathbf{x}^{n+1}_{(k+1)} - \mathbf{x}^{n+1}_{(k)} = \Delta t (\mathbf{v}^{n+1}_{(k+1)} - \mathbf{v}^{n+1}_{(k)})$$
$$\text{or} \quad \Delta \mathbf{x} = \Delta t \Delta \mathbf{v}$$

□

The linearization of equation (4.9) around $(\mathbf{x}^{n+1}_{(k)}, \mathbf{v}^{n+1}_{(k)})$ yields:

$$\begin{aligned}\mathbf{v}_{(k)}^{n+1} + \Delta\mathbf{v} &= \mathbf{v}^n + \Delta t \mathbf{M}^{-1}\Big(\mathbf{f}_e(\mathbf{x}_{(k)}^{n+1}) + \left.\frac{\partial \mathbf{f}_e}{\partial \mathbf{x}}\right|_{\mathbf{x}_{(k)}^{n+1}} \cdot \Delta\mathbf{x} \\ &\quad -\gamma \mathbf{K}(\mathbf{x}_{(k)}^{n+1})(\mathbf{v}_{(k)}^{n+1} + \Delta\mathbf{v})\Big)\end{aligned}$$

Note that this equation is not quite an exact linearization, because in the damping term we fixed the stiffness matrix at the value it had around configuration $\mathbf{x}_{(k)}^{n+1}$ instead of performing a first-order Taylor expansion. This modification leads to a much simpler (modified) Newton scheme for the Backward Euler system, and practically doesn't affect the convergence of the Newton scheme. We further manipulate the previous equation as follows:

$$\begin{aligned}\frac{1}{\Delta t^2}\mathbf{M}\Delta\mathbf{x} &= \frac{1}{\Delta t}\mathbf{M}(\mathbf{v}^n - \mathbf{v}_{(k)}^{n+1}) + \Big(\mathbf{f}_e(\mathbf{x}_{(k)}^{n+1}) \\ &\quad -\mathbf{K}(\mathbf{x}_{(k)}^{n+1})\Delta\mathbf{x} - \gamma\mathbf{K}(\mathbf{x}_{(k)}^{n+1})(\mathbf{v}_{(k)}^{n+1} + \frac{1}{\Delta t}\Delta\mathbf{x})\Big)\end{aligned}$$

$$\begin{aligned}\left[\left(1 + \frac{\gamma}{\Delta t}\right)\mathbf{K}(\mathbf{x}_{(k)}^{n+1}) + \frac{1}{\Delta t^2}\mathbf{M}\right]\Delta\mathbf{x} &= \\ &= \frac{1}{\Delta t}\mathbf{M}(\mathbf{v}^n - \mathbf{v}_{(k)}^{n+1}) + \Big(\mathbf{f}_e(\mathbf{x}_{(k)}^{n+1}) - \gamma\mathbf{K}(\mathbf{x}_{(k)}^{n+1})\mathbf{v}_{(k)}^{n+1}\Big) \\ &= \frac{1}{\Delta t}\mathbf{M}(\mathbf{v}^n - \mathbf{v}_{(k)}^{n+1}) + \Big(\mathbf{f}_e(\mathbf{x}_{(k)}^{n+1}) + \mathbf{f}_d(\mathbf{x}_{(k)}^{n+1}, \mathbf{v}_{(k)}^{n+1})\Big) \\ &= \frac{1}{\Delta t}\mathbf{M}(\mathbf{v}^n - \mathbf{v}_{(k)}^{n+1}) + \mathbf{f}(\mathbf{x}_{(k)}^{n+1}, \mathbf{v}_{(k)}^{n+1}) \qquad (4.10)\end{aligned}$$

The system described by equation (4.10) is symmetric and positive definite, and can be solved efficiently with a Krylov subspace method such as Conjugate Gradients. We also note that equation (4.10) only determines the update for the positions at time t^{n+1}. Velocities should be updated at each iteration using the relation $\mathbf{v}_{(k+1)}^{n+1} = \mathbf{v}_{(k)}^{n+1} + \frac{1}{\Delta t}\Delta x$.

As a final observation, equation (4.10) can be modified to yield a *quasistatic* simulation, where every configuration over time is the result of a rest configuration (subject to the imposed kinematic constraints and boundary conditions). We achieve this by setting $\Delta t \to \infty$, effectively indicating that at every simulated instance we allow infinite time for the elastic body to settle into an equilibrium configruation. The Newton iteration for this quasistatic problem simply becomes:

$$\mathbf{K}(\mathbf{x}_{(k)}^{n+1})\Delta\mathbf{x} = \mathbf{f}(\mathbf{x}_{(k)}^{n+1})$$

after which positions are updated as $\mathbf{x}_{(k+1)}^{n+1} \leftarrow \mathbf{x}_{(k)}^{n+1} + \Delta\mathbf{x}$.