Márton Solti

Interactive Finite Element Simulation of Deformable Objects

Master Thesis

Supervisor: Attila Kossa

Budapest University of Technology and Economics
Department of Applied Mechanics

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Young man, in mathematics you don't understand things.
You just get used to them.

– János Neumann (a.k.a *Good ole' Johnny*)

Budapest University of Technology and Economics
Faculty of Mechanical Engineering
Department of Applied Mechanics
http://www.mm.bme.hu/

FINAL PROJECT ASSIGNMENT

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Name: **Solti Márton**			ID: **71405767681**
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Details	1. General overview on continuum mechanics, finite element method and dynamics simulations. 2. Deformable objects in computer graphics - mass-spring systems, co-rotational FEM, invertible hyperelastic FEM. 3. Implement an interactive deformable object simulator. 4. Collision detection techniques, acceleration structures. 5. Rigid-body dynamics simulations. 6. Coupling of Rigid and Deformable bodies. 7. Summarize the results in English and in Hungarian. 8. Prepare a poster presentation of the work.
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Final Exam

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ZVEGEMMNWFE Finite Element Analysis	**ZVEGEMMNWAM** Advanced Mechanics	**ZVEGEMMNWCM** Continuum Mechanics	-

Authentication

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The undersigned declares that all prerequisites of the Final Project have been fully accomplished. Otherwise, the present assignment for the Final Project is to be considered invalid.

……..
Solti Márton

Abstract

The Finite Element Method (FEM) isn't just the core technology behind automotive innovation, but it's the fundation of many deformable object simulation techniques applied in movies and computer games. In this thesis, I review the use of FEM for volumetric deformable object simulations, but in the discipline of computer graphics.

After some introduction to nonlinear FEM and continuum mechnics, I present a generalized derivation of the tangent stiffness matrix, $\mathbf{K}$. Then, following Smith et al. in [25], I introduce a new, $\mathbf{S}$-based set of invariants: the Smith et al. invariants allow us the use of the rotation tensor $\mathbf{R}$ in the strain energy density functions in case of implicit methods by offering a closed form, analytic expression for the rotation gradient $\frac{\partial \mathbf{R}}{\partial \mathbf{F}}$.

In order to achieve interactive rates in a FEM simulator, we need to allow the use of large timesteps. However, this could produce a substantial divergence from the steady state, leading to a $\mathbf{K}$ that is often indefinite. This is a big problem as the fast, iterative linear system solver methods require a positive-definite system to converge. This problem is addressed by computing $\mathbf{K}$ from the eigenvalues $\mathbf{\Lambda}$ and eigenvectors $\mathbf{Q}$ as $\mathbf{K} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$, while not allowing the eigenvalues to be less than 0, thus keeping $\mathbf{K}$ positive-definite. For some energy density functions, the full eigendecomposition is available in closed form. This *'projection'* technique makes the simulation so robust that it recovers to the rest state even if it's crushed to a plane or a point.

Along the way I present some clever tricks applied in the industry, and in the end I implement an example simulator in C++ which is available at `marcisolti.github.io/ifem`.

Összefoglaló

A Végeselem Módszerrel (VEM) nem csak az autóiparban találkozhatunk: a filmekben és számítógépes játékokban található deformálható test szimulációk nagy része VEM-en alapul. Ebben a diplomamunkában térfogati deformálható testek szimulációját mutatom be, de főként a számítógépes grafika irodalmára támaszkodva.

A rövid VEM és kontinuum mechanika bevezető után egy általános tangens merevségi mátrix levezetési módszert ismertetek. Ezután mutatom be az $\mathbf{S}$-alapú, Smith et al. invariánsokat [25], amelyek lehetővé teszik a forgatási tensor $\mathbf{R}$ használatát alakváltozási energia-függvényekben implicit módszerek esetén is: forgatási gradiens $\frac{\partial \mathbf{R}}{\partial \mathbf{F}}$ zárt alakban elérhető segítségükkel.

Az interaktív szimulációk nagy időlépéseket ígényelnek, ez viszont gyakran vezethet indefinit $\mathbf{K}$-hoz. Ez nagy probléma, mivel a gyors, iteratív lineáris egyenletrendszer-megoldó módszerek csak pozitív definit mátrixokkal működnek. $\mathbf{K}$ pozitív definitté tehető, ha a sajátértékeiből $\mathbf{\Lambda}$ és sajátvektoraiból $\mathbf{Q}$ számítjuk $\mathbf{K} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$ segítségével úgy, hogy nem engedjük egyik sajátértékének sem, hogy negatív legyen. Több alakváltozási energia-függvény sajátérték és sajátvektor számítása elérhető zárt alakban. Ez a *"sajátérték vetítési"* technika lehetővé teszi, hogy egy síkba vagy pontba összenyomott végéselemes háló is visszanyerje eredeti alakját a szimuláció során.

Bemutatásra kerül még néhány, a szórakoztatóiparban alkalmazott egyszerű trükk, a dolgozat végén pedig egy minta-szimulátor C++ implementációját szemléltetem, amely a `marcisolti.github.io/ifem`-en is elérhető.

Declaration of independent work

I, Márton Solti, the undersigned, hereby declare that the present thesis work has been prepared by myself without any unauthorized help or assistance such that only the specified sources (references, tools, etc.) were used. All parts taken from other sources word by word or after rephrasing but with identical meaning were unambiguously identified with explicit reference to the sources utilized.

Márton Solti

Declaration of authorization

I authorize the faculty of Mechanical Engineering of the Budapest University of Technology and Economics to publish the principal data of the thesis work (author's name, title, abstracts in English and in Hungarian, year of preparation, supervisor's name, etc.) in a searchable, public, electronic and online database and to publish the full text of the thesis work on the internal network of the university (or for authenticated users). Full text of thesis works classified upon the decision of the Dean will be published after two years.

Done at Budapest, 10.06.2021.

Márton Solti

Glossary of Symbols

General Notation

Symbol	Description
$\mathfrak{R}$	set of real numbers
a	unbolded lowercase: scalar
$\mathbf{a}$	bold lowercase: vector
$\mathbf{A}$	bold uppercase: matrix
$\mathbb{A}$	blackboard bold: higher-order tensor
a_i	i^{th} element of a vector
a_{ij}	element in the i^{th} column and j^{th} row of some matrix
$\frac{\partial f}{\partial x}$	partial derivative of f in terms of x
$\text{vec}\,(\,\cdot\,)$	vectorization operation
$\|\,\cdot\,\|_F^2$	squared Frobenius norm
$\mathbf{U}$	left singular vectors of some matrix
$\mathbf{V}$	right singular vectors of some matrix
$\mathbf{\Sigma}$	singular values of some matrix
λ_i	i^{th} eigenvalue of some matrix
$\mathbf{q}_i$	i^{th} eigenvector of some matrix
$\mathbf{Q}_i$	i^{th} eigenmatrix of some tensor

Finite Element Method

Symbol	Description
$\mathbf{K}$	(tangent) stiffness matrix
$\mathbf{M}$	mass matrix
$\mathbf{C}$	damping matrix
$\mathbf{f}_{ext}$	nodal external forces
$\mathbf{f}_{int}$	nodal internal forces
Π	potential energy
$\Psi(\mathbf{F})$	strain energy density function
$\mathbf{u}$	nodal displacements
$\mathbf{x}$	spatial position $[x, y, z]^T$
$\dot{\mathbf{x}}$	velocity, a.k.a. $\frac{d\mathbf{x}}{dt}$
$\ddot{\mathbf{x}}$	acceleration, a.k.a. $\frac{d^2\mathbf{x}}{dt^2}$
h	timestep size
v	volume of a volumetric element
a	area of a shell element

Continuum Mechanics

Symbol	Description
$\mathbf{x}$	spatial coordinate
$\mathbf{x}$	no overline: a value ($\mathbf{x}$) at the *material* configuration
$\overline{\mathbf{x}}$	with overline: a value ($\mathbf{x}$) at the *spatial* configuration
ϕ	motion
$\mathbf{F}$	deformation gradient
$\mathbf{C}$	right Cauchy-Green deformation tensor
$\mathbf{E}$	material Green-Lagrange strain tensor
$\mathbf{R}$	rotation tensor
$\mathbf{S}$	right stretch tensor
J	volume change
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\mathbf{P}$	first Piola-Kirchhoff stress tensor
I_{C}	first Cauchy-Green invariant
II_{C}	second Cauchy-Green invariant
III_{C}	third Cauchy-Green invariant
I_1	first Smith et al. invariant
I_2	second Smith et al. invariant
I_3	third Smith et al. invariant
μ	Lamé's first parameter
λ	Lamé's second parameter

Contents

Chapter 1

Introduction

Did you know that simulating deformables with the Finite Element Method (FEM) is also pretty popular in the entertainment industry as well? Yes, the same FEM we all know very well, is behind all the cloth and hair simulations, character animations we see in those Hollywood blockbusters and AAA games.

This thesis is about the application of FEM, but in the discipline of computer graphics. In the old days, physics simulation in computer graphics – in movies and games – was about creating *physically plausable* visual effects with some smart tricks – *hacks*. The field of deformable simulation advanced greatly in the last few decades: researchers built upon the FEM techniques found in mechanical engineering literature while bringing some exciting innovations to the field as well.

The thesis' title is *interactive* FEM simulation of deformables, which might suggest that this whole text will be about bit hacks and weird x86 assembly instructions. You usually have to wait, when you run a simulation in ANSYS, right? How do you make this interactive? Of course, the *implementation* is equally important in this case, but we will look at the *math* behind the sheer *craftsmanship* of high performance simulator programming instead.

First we will go through the basic concepts of computer graphics and animation, FEM, and continuum mechanics in Chapter 2-4. Then we will start our journey into the ins and outs of interactive volumetric simulations in the field of computer graphics. Just to offer you a spoiler, we will look deeply into the efficient computation (Chapter 5) as well as the *stability* (Chapter 6) of the tangent stiffness matrix $\mathbf{K} = \frac{\partial^2 \Psi(\mathbf{F})}{\partial \mathbf{x}}$, mostly following the work of Pixar Research. (Smith et al. in [24], [25] and [15]) We were able to implement a super-robust quasistatic simulator (Chapter 8) which recovers to the rest state even if the whole mesh is squished into a plane or a point (Chapter 9). Along the way we will look at some clever tricks applied in the industry (Chapter 7).

The supplementary materials are available at `marcisolti.github.io/ifem`. This includes the full source code, as well as some videos of the implemented sample simulator.

Chapter 2

Computer Graphics and Animation

2.1 Computer Graphics

Computer Graphics is an umbrella term for any method that is about synthesizing and manipulating visual content. Major subfields include:

- **Geometry** processing, or *computational geometry*, which is about the representation and processing of surfaces. We will look at some examples from this subfield, as FEM is pretty popular there.
- **Rendering**, or *image synthesis* is about telling what color should each pixel be. Rendering usually simulates the physics of light in order to create realistic images.
- **Animation** is about the description of geometry, that *move or deform over time*. It's basically describing a geometry, but in 4D.

2.1.1 A typical scene

Let's describe a typical example of creating a computer generated image of a *3D scene*, pictured on Fig. 2.1. A *scene* contains all the resources and models that participate in the image synthesis. It's the whole thing on Fig. 2.1.

In order to *draw* an image of this scene with the computer, we need to simulate all the photons that would get into our eye, if we were to look at the same scene in real life (IRL). *Image synthesis* – a.k.a. *rendering* – is all about that. It simulates the physics of light: photons are emitted from the *light sources* bounce around the scene. They interact with the surfaces on the way, and eventually hit our digital *eye*, determining what color a pixel should be.

The set of surfaces that are present in the scene – i.e. the drawable models' *geometry* – are usually defined as a *set of triangles*. The surfaces' material defines how light's interacting with it, which also determines how it's going to look like: is it a shiny silver one, or is it matte black? The interaction – and the look, or the *shading* – will be very different. There have been thick books written about how light's interacting with different surfaces, e.g. [20]. When you hear *shader code*, it's usually some code running on the GPU, calculating the result of some specific surface interaction.

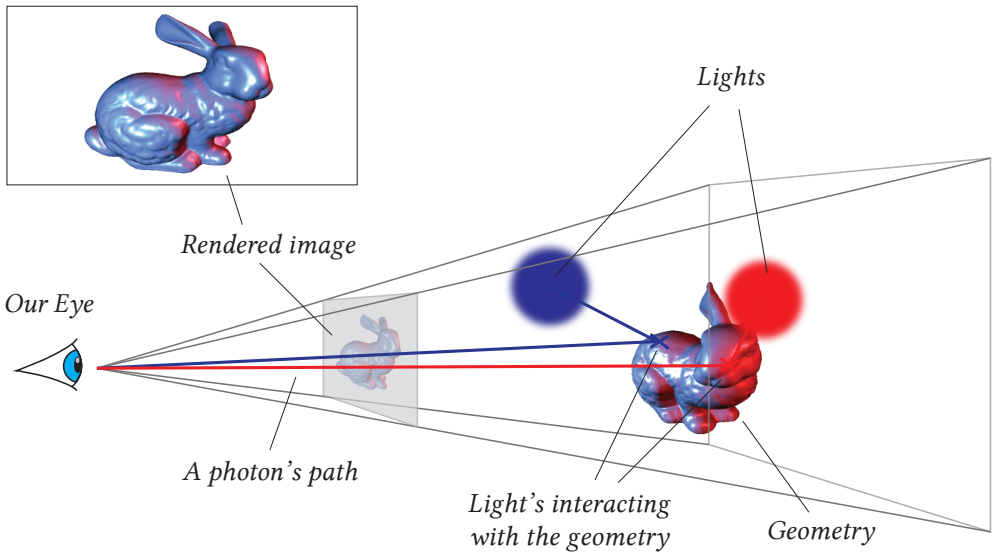

Figure 2.1: A typical *scene*

2.1.2 Real-Time vs. Offline

A thing we have to make clear in the beginning, is the difference between *real-time* and *offline* simulations.

A *real-time* simulation means that the solution is *running real-time*: each frame of data is calculated *'on the fly'*, right before the image is shown on the screen. This usually means that we have a specific amount of time to calculate *everything* – $1/30 = 0.0333$ s if we display 30 images per second, or $1/60 = 0.0167$ s if we display 60 images a second. Good examples for real-time solutions are games, of course, but there is a vast field of applications outside of the entertainment industry, like simulators for training professionals – e.g. forklift operators or fighter jet pilots.

Offline simulations on the other hand, are usually for stuff that is *not* feasible for real-time. In case of rendering, while real-time graphics is for games, offline rendering is for animated movies and CGI effects. However, they use fundamentally different methods to simulate light.

2.2 Animation

We talked about *geometry* and *rendering* a lot, but haven't said a word about *animation* since I introduced it. Animation is essentially about describing geometry, but in *time* as well – so instead of $[x, y, z]^T$ we have $[x, y, z, t]^T$

Usually, an artist – an animator – creates the animation with some animation software – like Maya. However, a typical mesh's vertex count is in the magnitude of thousands – millions. Would an artist move all these points by hand? It *certainly* is a possibility, but most of the time it would be stupid, and we need a *more optimal* (sic!) way. One key method to mention here is *skeletal animation.*

Skeletal animation (Fig. 2.2) is usually used in character animation, where a character has two representations: a surface representation used to draw the character (called the mesh or skin) and a hierarchical set of interconnected parts (called bones, and collectively forming the skeleton or rig),

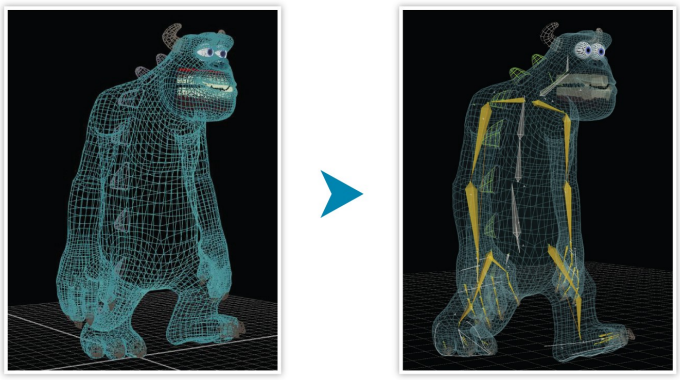

Figure 2.2: Skeletal animation [21]

a virtual armature used to animate the mesh: the position of these bones are set for some specific points in time – called *keyframes* – and the software *interpolates* between the keyframes in some manner.

2.3 Physically Based Animation

What about other kinds of animations? E.g. imagine you want to animate a realistically moving curtain. How do you do that? You can *certainly* do it by hand, but it would probably cost hundreds of hours of work.

Why not just simulate it? Isn't it just some FEM simulation at the end of the day? The answer is yes, such a *cloth simulation* is *nothing but* a FEM simulation. The area of physics simulation based animations is usually called Physically Based Animation.

Physically Based Animation includes every type of animation what's done by simulating some physical phenomena. Important examples include:

- **Rigid Body Dynamics** is the same rigid body dynamics we talk about in computational mechanics, in our case however, this is done usually in a real-time, interactive framework. Good examples of such frameworks are *PhysX* and *Havok*. It has to be noted that
- **Collision Detection**, the act of detecting the intersection of two or more objects, is an equally important part of rigid body dynamics frameworks. Two main engineering challenges are:
  - First you have to find explicit formulas for figuring out if two pieces of geometries intersect or not. Notable methods include the Gilbert–Johnson–Keerthi distance algorithm [7].
  - Just to elaborate on this a bit: how will you know if any of n objects would intersect with any other object in the scene? The naive way would be to check every other object, if they're intersected by the one in question. That's at least n^2 steps –
    – which could be a lot! We will need to optimize this, and the *'basic approach'* is to build some spatial acceleration structure, where we could discard almost all elements from the problem.

- **Simulation of Fluids** – be it liquid or even sound – is usually done the usual way, by approximating the Navier-Stokes equation on a Cartesian grid. However, Eulerian and hybrid methods are definitely on the rise with the (re)introduction of the Material Point Method by the Disney Research Team: in [30] they proposed a new method for simulating snow. (Fig. 2.3a)

- **Deformables** – just like fluids – is done the usual way, using FEM. However there are notable exceptions, pushing a (semi-)particle-based solver, e.g. the aformentioned Material Point Methods [30] or Position Based Dynamics [19].

2.4 Physically Based Deformables

In 1987, Terzopoulos et al. introduced elastically deformable objects to the computer graphics community in a seminal paper [34]. Since then, numerous researchers have partaken in the quest for the visually and physically plausible animation of deformable objects.

Your natural engineering instinct might suggest that there has to be some trick involved in the models used by deformables in this field. There are a few clever tricks indeed, some of them are presented along the way in this text, but by and large, we are talking about the same *'basic'* FEM and continuum mechanics we all know and love.
Notable examples from the industry:

- **Cloth Simulation** was the original problem which sparked innovation in the late 90s. Everyone in the field knows the original Baraff-Witkin paper [2]. The method presented there was used to simulate Boo's T-Shirt in Monsters Inc. (See Fig. 2.3b)

- **Character Animation** is another field which was pioneered by Pixar using FEM. They were the first to use a sophisticated volume simulation, in order to simulate the fleshy behaviour of an animated character's flesh. (Fig. 2.3c) More specifically, they were not able to model Mr. Incredible's (2004) muscular body with their existing linear interpolation scheme, so they had to design a completely new solution, based on nonlinear FEM and a hyperelastic constitutive model [11].

- Have you noticed how great **Hair Simulations** has become? Disney Research is the big player in the hair game [14]. Aside from their supreme physically based hair simulation, they have a very intuitive toolset which allows the artist to art-direct the movement of hair. (Fig. 2.3d)

- This new paper by Facebook Reality Labs [26] is so great that I have to make a separate point for **Hand Physics**. Hand physics deals with the real-time simulation of the user's hands in virtual reality. Smith et al. achieve an *epic* hand model by constraining a vision-based tracking algorithm with FEM, using a Neo-Hookean constitutive model. Their algorithm is able to handle self-interaction like massaging of the hands. (Fig. 2.3e)

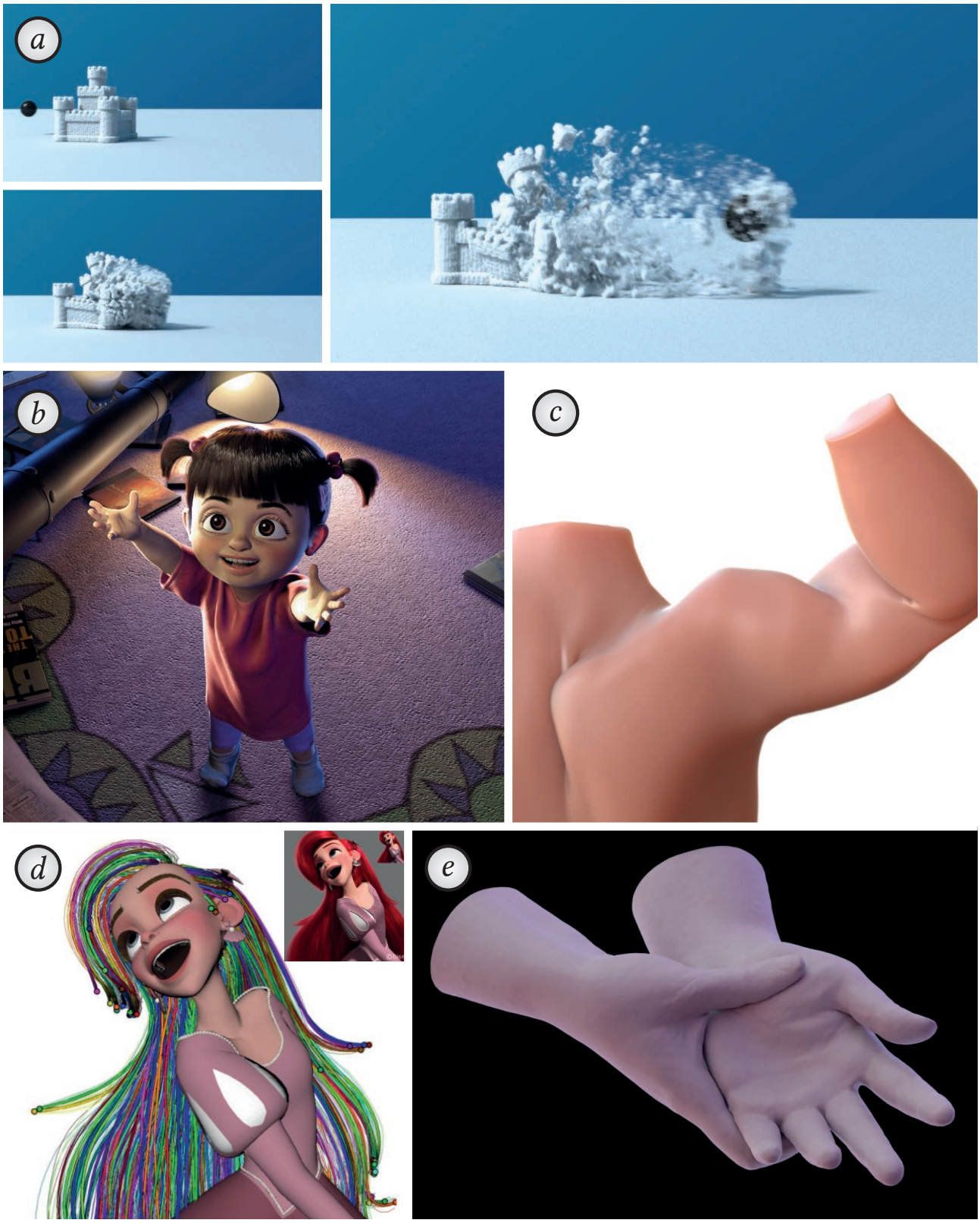

Figure 2.3: Examples of Physically Based Animation: a – Material Point Method for snow simulation [30]; b – Implicit backward Euler formulation for cloth simulation [2]; c – Stable Neo-Hookean flesh simulation for character animation [24]; d – Art-directed hair simulation [14]; e – Constraining dense hand surface tracking with elasticity for VR hands [26];

Chapter 3

Fundamentals of FEM

3.1 The Essence of FEM

The Finite Element Method (FEM) is the core technology behind many applications for engineering analysis. Despite that we are *'just'* going to use it for some Physically Based Animation, the math and physics behind it stays the same.

3.1.1 The Lumped-Paramter Mathematical Model

Just to be sure we are talking about the same FEM, let's walk through the fundamentals of it. I think the best summary is the definition of *'lumped-parameter mathematical models'* by Bathe in [5]:

"The essence of a lumped-parameter mathematical model is that the state of the system can be described directly with adequate precision by the magnitudes of a finite (and usually small) number of state variables. The solution requires the following steps:

1. ***System idealization:*** *the actual system is idealized as an assemblage of elements.*
2. ***Element equilibrium:*** *the equilibrium requirements of each element are established in terms of state variables*
3. ***Element assemblage:*** *the element interconnection requirements are invoked to establish a set of simultaneous equations for the unknown state variables*
4. ***Calculation of response:*** *the simultaneous equations are solved for the state variables, and using the element equilibrium requirements, the response of each element is calculated."*

In this section, we are going to elaborate on this definition according to Fig. 3.1.

Idealization

According to this definition, we need to *idealize the system* first. This means that we relaxate the problem a bit, we make some assumptions and simplifications in order to make the problem computable. This is most important part.

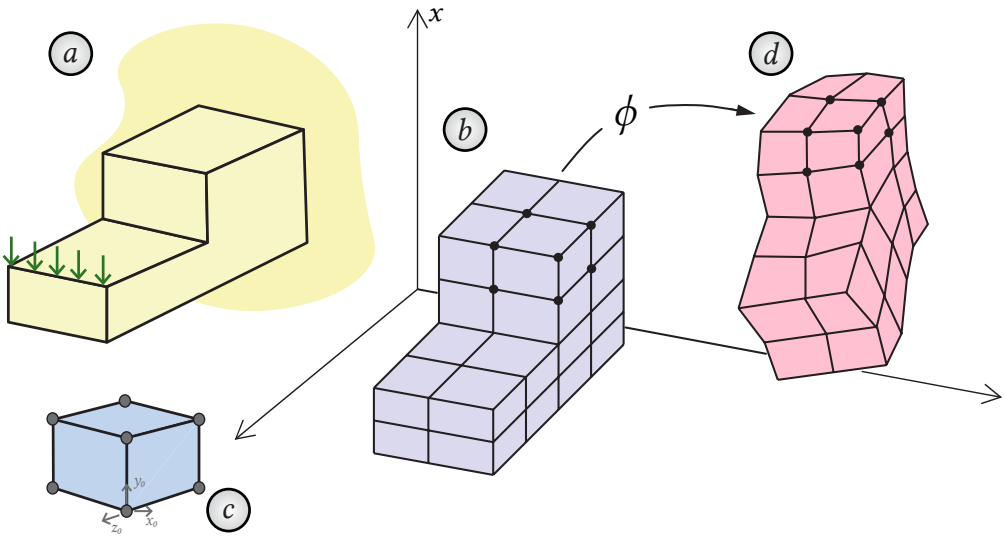

Figure 3.1: a - Modelling the physical phenomena of a deformable object having one end built in to the wall, while the other end is loaded with some forces. b - The problem is idealized as a set of brick elements (c). d - the response of the set of elements – the movement of the all the nodes, ϕ – is calculated according to the loads/boundary conditions.

In order to do so, first we need to figure out what kind of problem we are dealing with. Are we doing a fluid simulation? A simulation of dynamic deformables? Maybe a coupled fluid-deformable sim? All of them are possible.

On Fig. 3.1, you can see a neat example of system idealization: instead of integrating the fundamental equations of elasticity through that L-shaped thing *(a)*, we build an L-shaped thing *(b)* from small bricks *(c)*, with which we can compute stuff much easier.

State Variables, Element Equilibrium

The problem in discussion determines what kind of elements we are going to use. The structural elements are the atomic building blocks of FEM. We define structural elements, whose behaviour can be fully characterized and understood. We then use these elements to build much more complex structures – just like on Fig. 3.1.

The structural elements' behaviour – or *response* – is characterized by a set of *state variables*. The ideas of the *response* and *state variables* are much easier to digest through an example, so let's look at the response of a structural element: a linear elastic spring. (Fig. 3.2)

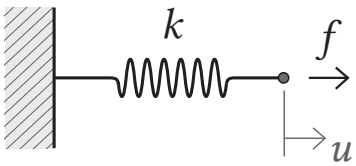

Figure 3.2: A linear elastic spring with single degree of freedom

The *response* of a spring with *linear spring-characteristics*, that has one of its ends attached to some fixed object, while the other end is pulled by some force of magnitude f, is calculated as

$$ku = f, \tag{3.1}$$

This is the element equilibrium! Here the *response* is the displacement of the pulled end, denoted by u. u is the state variable! k on the other hand, is the *spring constant*. k is a positive, real number; it can be thought as the material property of the spring. k and u together completely characterizing the response – or *behaviour* – of this ideal spring.

Loosely speaking, f can be thought as some external *'energy'* which *'perturbates'* the system from its steady state. As a response, the system *'stores'* this energy in the spring itself, by equilibrating f with ku, hence the equation $ku = f$.

Global Stiffness Matrix Assembly, Calculation of the Response

Now we've got our state variables and structural elements defined, and we also have some notion as to what the system's response is. All that's left is to elaborate a bit on the element assemblage and the calculation of its response.

In order to build some structures from the structural elements, we need to define how they are connected together. This is done by accumulating each individual elements' *'behavioural data'* in the *global stiffness matrix* $\mathbf{K}$ using the *direct stiffness method*. The process is explained later in Sec. 3.1.3, but what we are doing is essentially expanding the idea of the $ku = f$ for an n dimensional problem, such that

$$\boxed{\mathbf{Ku} = \mathbf{f}_{ext}.} \tag{3.2}$$

Here we stacked all the state variables in a vector $\mathbf{u}$, which denotes each elements' displacement, while the external forces are stacked in the same manner in $\mathbf{f}_{ext}$; both $\mathbf{u}$ and $\mathbf{f}_{ext}$ are $\in \mathfrak{R}^n$. The global stiffness matrix $\mathbf{K} \in \mathfrak{R}^{n \times n}$ is characterizing the *system's response as a whole*.

Plugging in any force vector $\mathbf{f}$ to 3.2 results in a nice linear system which we can solve for $\mathbf{u}$. So cool! And actually Eq. 3.2 is the fundamental equation of FEM; basically we always want to solve this very equation. But where does this $\mathbf{K}$ come from?

You probably know the answer already, and have a hard time not to fall asleep reading this chapter. If it's not the case, I recommend you to read Appendix A, where I go through an easy example wrapping all the things up presented in this section.

3.1.2 Structural Elements

The structural elements represent the fundamental building block of FEM. The state variables are usually some spatial points called nodes; an element that connects some nodes together. The different elements are connected together with these nodes. In the simulations, we solve the equation $\mathbf{Ku} = \mathbf{f}_{ext}$ for the nodal displacements $\mathbf{u}$, and interpolate the results to aquire the values inside the element. You can find some elements on Fig. 3.3.

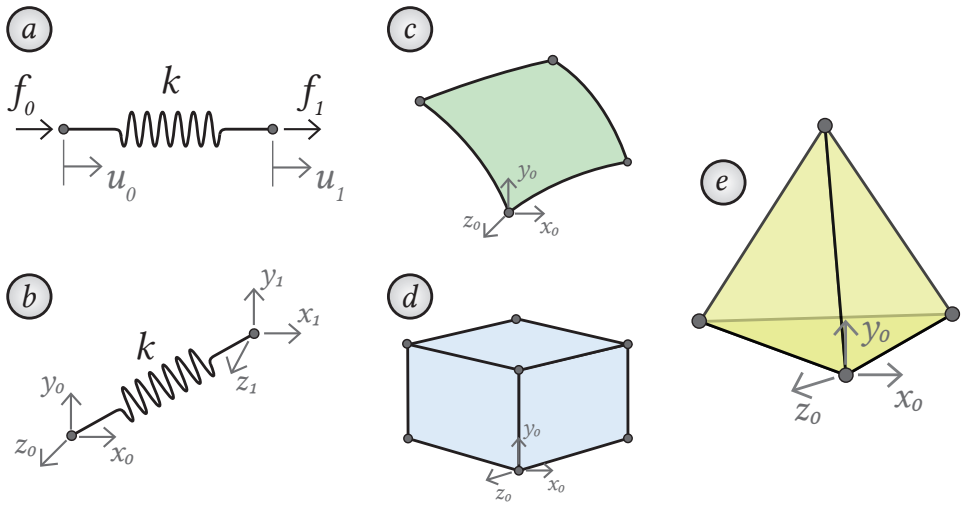

Figure 3.3: Different Structural Elements

We define structural elements, whose behaviour can be fully characterized and understood, and use these elements to build much more complex structures. This is done by accumulating each individual elements' *'behavioural data'*in the global stiffness matrix. This *'behavioural data'* is in the form of *element stiffness matrices*.

1D elements

In case of some special structures, like trusses and beams, *element stiffness matrices* can be aquired in closed form. Let's derive the stiffness matrix of the *1D truss element* as of Fig. 3.3a. This is pretty much $ku = f$ again, but the equilibrium now is a *system of equations*

$$\begin{aligned} k(u_0 - u_1) &= f_0, \\ k(-u_0 + u_1) &= f_1, \end{aligned} \tag{3.3}$$

which can be reformulated as

$$k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \end{bmatrix}. \tag{3.4}$$

In this equation

$$k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} = \mathbf{K}^{(e)}, \tag{3.5}$$

is the *element stiffness matrix of the 1D truss element.* Actually, we would get back our *rank-1* $ku = f$ with $u_0 = 0$ and $u_1 = u$. Nice! And this idea scales pretty well to *3D truss elements*, like the one on Fig. 3.3b.

Two- and Three-Dimensional Elements

The big picture is that you are essentially doing the same thing with continuous structures: you can build 2D structures from 2D elements, like the quad element on Fig. 3.3c; and 3D structures from 3D, volumetric elements, like the hexa *'brick element'* on Fig. 3.3d or the classic tetrahedron a.k.a. tet on Fig. 3.3e. However, the math is very different behind it!

In the analysis of some *'1D'*, beam or truss structures, the exact element stiffness matrices can be calculated. The stiffness properties of a beam element are physically the element end forces that correspond to unit element end displacements – in beam theory!

However, if we consider more general, 2D or 3D continuous structures, we need to use a very different approach to approximate the actual displacements. The reason is that we do *not* know the exact displacement functions opposed to the case of truss and beam elements. The result is going to be a set of *partial differential equations*, whose equilibrium are not satisfied in general, but this error is reduced as the finite element idealization of the structure or the continuum is refined.

There are many ways to derive these differential equations in discussion, that are more specifically the general formulation of the finite element method. In this text, we are going to approach it as a *minimization of the total potential of the system*; presented later on in Sec. 3.2.

3.1.3 The Direct Stiffness Method

Quick recap: the basic process is that the complete structure is idealized as an assemblage of individual structural elements. We now have some understanding of what the elemental stiffness matrices are.

The next step is to assemble the global stiffness matrix $\mathbf{K}$, characterizing the system as a whole. The *direct stiffness* method states that the global stiffness matrix $\mathbf{K}$ can be calculated by summing up the element stiffness matrices:

$$\mathbf{K} = \sum_{i}^{n} \mathbf{K}^{(i)}, \tag{3.6}$$

where n is the number of element, and $\mathbf{K}^{(i)}$ is the i^{th} element's stiffness matrix, but *expanded in the dimensions of the global degrees of freedom* by filling in zeros at positions related to nodes not adjacent to the element.

In order to consolidate this idea together with the whole lumped-parameter mathematical process, let's consider a new example, shown on Fig. 3.4.

3.1.4 Example: Mass-Spring Systems

Believe it or not, most deformable simulations of cloth and volumetric objects were based on the simple spring model I presented in this section. Instead of integrating the proper finite element formulation, they just built some approximate structures from masses and springs, called – not so suprisingly – Mass-Spring Systems. You can see a neat example at Fig. 3.5.

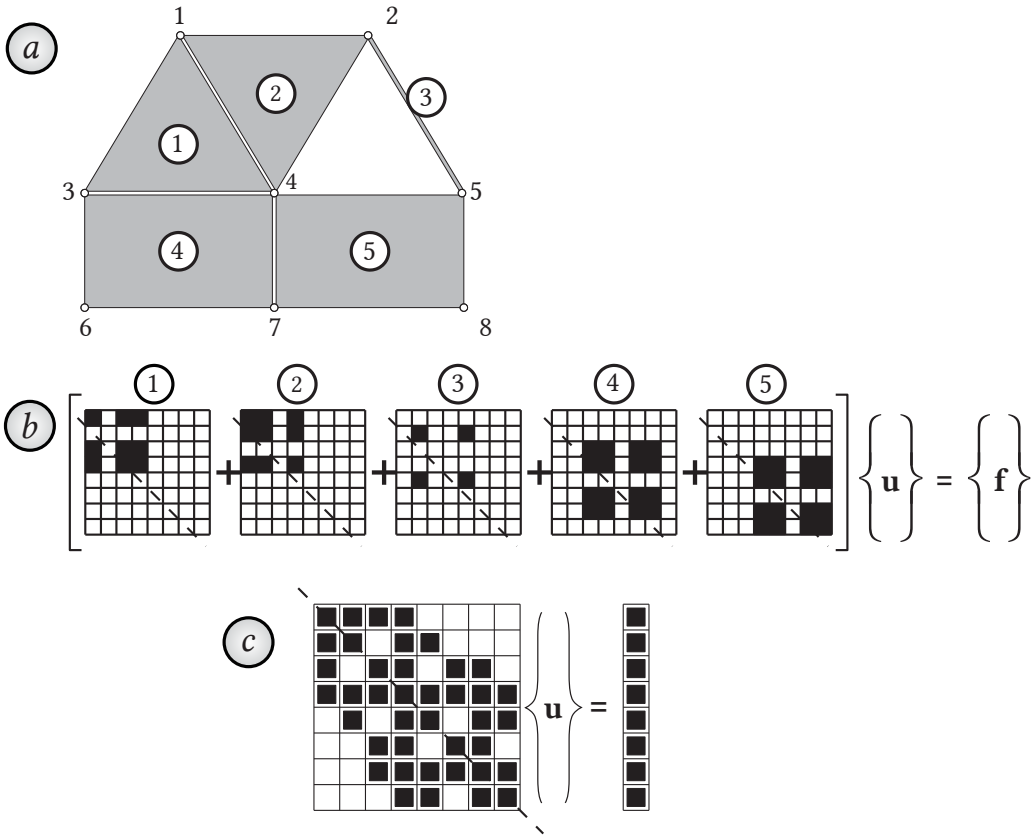

Figure 3.4: The general pattern: a – The system is an assemblage of structural elements. b – Element stiffness matrices are formulated. c – The element stiffness matrices are accumulated to the global stiffness matrix by adding the element matrix to the corresponding degrees of freedom, according to the element interconnection [36]

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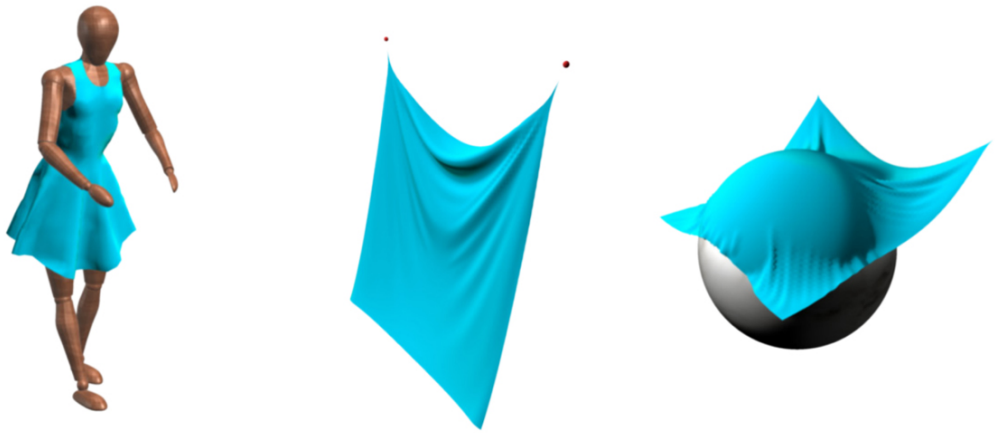


Figure 3.5: Mass-Spring Simulation of cloth [16]

.

Despite its simplicity, you can make pretty nice sims with such a simple formulation as well. Just take a look at Fig. 3.5: Mass-Spring simulation of cloths could work really well. There is a catch of course: this is *not* how cloth's physics work at all. You have to tweak some *'arbitrary'* parameters to get the *'visual effect'* you want to achieve. That is why I would not call this a *physically based* method.

3.2 Finite Element Formulation

For the *'proper'* finite element formulation pretty much need to do the same thing what we did in the analysis of truss structures: first we need to idealize the structure as an assemblage of elements. The only difference is that the elements are going to abstract some 2D or 3D continuum – we've already talked about this in Sec. 3.1.2. In the end, we are going to end up with the same element stiffness matrices, that can be accumulated in the same manner – with the direct stiffness method – in the global stiffness matrix. However, it will take some work to make the calculation of the element stiffness matrices equally easy and pretty. Don't be afraid, we will end up with the same, comfortable $\mathbf{Ku} = \mathbf{f}$. We'll start our journey with the law of conservation of energy.

3.2.1 Conservative Systems

The law of conservation of energy states that the total energy of an isolated system remains constant. You can loosely state this as

$$\sum \Pi = \text{const}, \tag{3.7}$$

where Π is some conservative – or *potential* – measure. E.g. chemical energy is converted to kinetic energy when a stick of dynamite explodes.

From basic calculus we also know, that if a function is constant, its derivatve must be 0, that is

$$\frac{\partial \Pi}{\partial \mathbf{x}} = 0. \tag{3.8}$$

This is a very important property!

Likewise, a very important property of a conservative force field is that it's independent from the path taken. Let's consider a more pacifist example. We drop a bowling ball – or a feather – located at $\mathbf{x} = [x, y, z]^T$ down a huge vacuum chamber. The only force we reasonably expect to act on the body is the gravitational field, which is a conservative measure. The body has potential energy $\Pi(\mathbf{x}) = m\mathbf{g}\mathbf{x}$ where $\mathbf{g} = [0, 0, g]^T$. Now, following Eq. 3.8 we can then obtain the gravitational force as the negative gradient of the potential energy with respect to the object position $\mathbf{x}$:

$$\mathbf{f} = -\frac{\partial \Pi}{\partial \mathbf{x}} = [0,\ 0,\ -mg]^T. \tag{3.9}$$

3.2.2 Balance of Total Potential Energy

Let's go back to deformables, and try to apply this idea to them. First, we need to postulate that we only consider conservative energies. Consider it done!

If the internal potential energy Π_{int} in a deformable object is aggregated in the system by some external source Π_{ext}, we can state that

$$\Pi_{int} + \Pi_{ext} = \text{const.} \tag{3.10}$$

So far, so good! Now going back to the *lumped-parameter mathematical model* (Sec. 3.1.1), we'll need to find some *state variables* in order to calculate the *response* of the system.

In case of *'highly deformable'* deformables, we're approaching *continuum mechanics* territory. Continuum mechanics is a separate discipline on its own, dealing with the mechanical behaviour of materials modeled as a continuous mass. Chapter 4 is all about the fundations of continuum mechanics, so let's just cut to the chase now.

Our state variable is going to be the *deformation gradient* $\mathbf{F}$. It is calculated for each continuum element, and all you need to know now that it quantifies how much deformation – rotation and scaling – that element has sustained. We are going to exclusively write all calculations in terms of $\mathbf{F}$, so it's hard to overstate its importance.

We got our state variables; what do we do with them? This is a really hard question to answer. Intuitively, the question is more like: if we squash the element *some amount*, *how much energy does it generate*? If I squash it just a little bit, the system should probably *'contain less energy'* compared to crushing it completely to the point that it becomes a pancake.
In actuality, these are two separate questions:

1. How squashed am I? Or: how badly deformed am I compared to my original shape? We already answered that: the deformation gradient $\mathbf{F}$ measures this quality.

2. How much energy does this cost? Once I know exactly how deformed I am, what should I do with this knowledge?

In order to answer this question, we need to exploit the fact that we are talking about a conservative system. In this case the energy is fully determined by the deformation gradient, and it has a special name: strain energy. An alternative definition could state that the consequence of elastic deformation is the accumulation of strain energy.

The measure we are going to use is the strain energy density function $\Psi(\mathbf{F})$. It assigns a deformation score for a corresponding $\mathbf{F}$, which is a number, so if you want to sound like a true intellectual, you can call it a *scalar valued tensor function*. Ψ measures the *strain energy per unit undeformed volume* on an infinitesimal domain dV. Integrating through the entire body Ω_0 yields the total potential energy of the system:

$$\Pi_{int} = \int_{\Omega_0} \Psi(\mathbf{F}) dV. \tag{3.11}$$

I don't know if it's just me, but I tend to get pretty anxious when I see an integral. We are lucky because there's a pretty intuitive way to get rid of it, presented in Sec. 7.1. We will use a special case of a tetrahedron with piecewise linear bases, with a single quadrature point in the center of it. In this case Eq. 3.11 becomes

$$\Pi_{int} = v\Psi(\mathbf{F}), \tag{3.12}$$

where v is the volume of the tetrahedron. This is so easy that literally every computer graphics article that uses some kind $\Psi(\mathbf{F})$-based continuum mechanics measure uses the formulation I present in Sec. 7.1.

Can we finally get the formula for $\mathbf{K}$? Bear with me for a couple more loops, and focus on a new physical concept instead: the *internal elastic force* incurred by a given deformation is calculated in the same manner as the bowling ball – vacuum chamber example in Eq. 3.9:

$$\mathbf{f}_{int} = -\frac{\partial \Pi_{int}}{\partial \mathbf{x}} = -v\frac{\partial \Psi}{\partial \mathbf{x}}. \tag{3.13}$$

This is the force that pushes back on you when you squash a tetrahedron! This is a set of nonlinear equation, and we are going to *'solve'* them the way such a set of equations should be *'solved'*: with the Newton-Raphson Iterative Scheme.

3.2.3 The Newton-Raphson Iterative Scheme

The Newton-Raphson method is an iterative scheme, which produces successively better *approximation* of a real-valued function's roots. See Fig. 3.6 for a nice visualization.

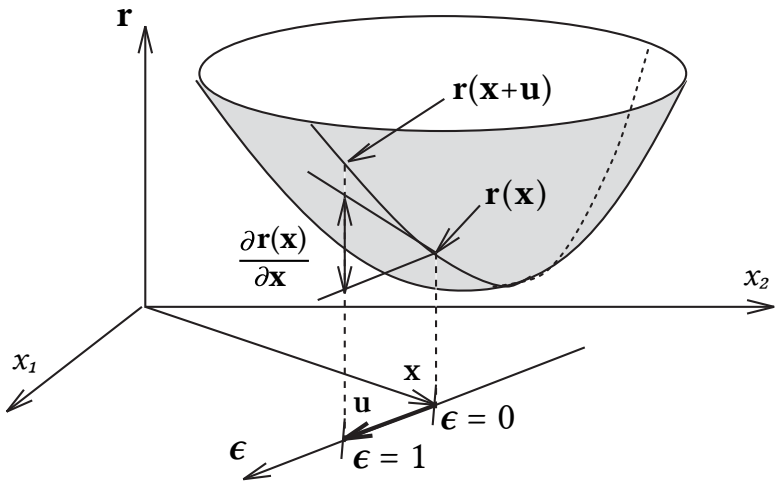


Figure 3.6: The Newton-Raphson scheme.

Consider the solution of a set of nonlinear algebraic equations:

$$\mathbf{r}(\mathbf{x}) = \mathbf{0}, \tag{3.14}$$

where, for example, a simple case with two equations and two unknowns is:

$$\mathbf{r}(\mathbf{x}) = \begin{bmatrix} r_1(x_1, x_2) \\ r_2(x_1, x_2) \end{bmatrix}. \tag{3.15}$$

In the Newton–Raphson iterative process, we have some solution estimate $\mathbf{x}_k$ at iteration k. The value of the next iteration $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{u}$ is obtained in terms of an increment $\mathbf{u}$ by establishing the linear approximation

$$\mathbf{r}(\mathbf{x}_{k+1}) \approx \mathbf{r}(\mathbf{x}_k) + \frac{\partial \mathbf{r}(\mathbf{x}_k)}{\partial \mathbf{x}} = 0. \tag{3.16}$$

The directional derivative $\frac{\partial \mathbf{r}(\mathbf{x}_k)}{\partial \mathbf{x}}$ is evaluated with the help of the chain rule as

$$\begin{aligned} \frac{\partial \mathbf{r}(\mathbf{x}_k)}{\partial \mathbf{x}} &= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \mathbf{r}(\mathbf{x}_k + \epsilon \mathbf{u}) \\ &= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \begin{bmatrix} r_1(x_1 + \epsilon u_1, x_2 + \epsilon u_2) \\ r_2(x_1 + \epsilon u_1, x_2 + \epsilon u_2) \end{bmatrix} \\ &= \hat{\mathbf{K}}\mathbf{u}. \end{aligned} \tag{3.17}$$

You might have noticed, that for a given $\mathbf{x}$ and $\mathbf{u}$, $\mathbf{r}(\mathbf{x}_{k+1})$ is the function of the parameter ϵ and we just derived the first-order Taylor series expansion about $\epsilon = 0$. Cool!

However, there's a much more important thing about Eq. 3.17. Matrix $\hat{\mathbf{K}}$ is the *tangent matrix* of the system:

$$\hat{\mathbf{K}} = \frac{\partial \mathbf{r}}{\partial \mathbf{x}}. \tag{3.18}$$

If we substitute Eq. 3.17 for the directional derivative into Equation Eq. 3.16, we obtain a linear set of equations for $\mathbf{u}$ to be solved at each Newton–Raphson iteration as

$$\hat{\mathbf{K}}\mathbf{u} = -\mathbf{r}, \quad \mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{u}. \tag{3.19}$$

If we plug in the principle of total potential energy into 3.19, we will finally, *FINALLY* get our hands on this precious $\mathbf{K}$. However $\mathbf{r} \neq \Pi_{int} + \Pi_{ext}$, but

$$\mathbf{r} = \frac{\partial \Pi_{int}}{\partial \mathbf{x}} + \frac{\partial \Pi_{ext}}{\partial \mathbf{x}} = \mathbf{f}_{int} - \mathbf{f}_{ext}. \tag{3.20}$$

It's because the derivative is the one that should be zero – following Eq. 3.8.

We haven't really talked about Π_{ext} much, what's the deal with that? This is because if you use exclusively nodal forces – forces explicitly only acting on the nodes – in your simulator, Π_{ext} burns away during differentiation, so you don't need to worry about it, just add it to the final $\mathbf{Ku} = \mathbf{f}$ system and you're done. You can definitely go fancy and define some more exotic external energies, like external pressure components as in [6] Example 9.6; however, they might contribute to you tangent matrix as they may *not* burn away with differentiation.

Consequently, by plugging in $\mathbf{r} = \mathbf{f}_{int} + \mathbf{f}_{ext}$ into Eq. 3.19 we've arrived at our final set of equations: when only nodal forces are considered, the *tangent stiffness matrix* $\mathbf{K}$ is defined as

$$\boxed{\mathbf{K} = -v\frac{\partial \mathbf{f}}{\partial \mathbf{x}},} \tag{3.21}$$

where I've dropped the *int* subscript for brevity. Many texts do that. There is an alternative form

$$\boxed{\mathbf{K} = -v\frac{\partial^2 \Psi}{\partial \mathbf{x}^2},} \tag{3.22}$$

which is at least as important as the $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$ form. It expresses that while the force is the energy *Jacobian*, the tangent stiffness matrix is the energy *Hessian*. In this text I use all three terms.
The Newton-Raphson iteration step is then defined as

$$\boxed{\begin{aligned}\mathbf{K}\mathbf{u} &= -\mathbf{f}_{int} + \mathbf{f}_{ext},\\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \mathbf{u},\end{aligned}} \tag{3.23}$$

where again

$$\boxed{\mathbf{f}_{int} = -v\frac{\partial \Psi}{\partial \mathbf{x}},} \tag{3.24}$$

so you can pretty much write this slightly more obtuse form as well:

$$-v\frac{\partial^2 \Psi}{\partial \mathbf{x}^2}\mathbf{u} = v\frac{\partial \Psi}{\partial \mathbf{x}} + \mathbf{f}_{ext}. \tag{3.25}$$

We've just defined the *quasistatic formulation* of the nonlinear finite element procedure. I will be telling you in the next section why it's called the quasistatic formulation, but let me calm you down a bit if you've got a bit afraid of these mysterious Hessians and Jacobians.

There is surely a lot of here to digest, but believe me, everything will become so clean and pretty, you will be dying to program your first simulator after you've finished reading my thesis. The thing is that you *really* just have to take the derivative; that's it! There *are* of course lots of evil professor tricks lurking around here, but all of them are going to be addressed in my favourite chapter, Chapter 5.

3.3 Dynamics Simulation

Believe it or not, we pretty much defined the key equation ($\mathbf{K}\mathbf{u} = -\mathbf{f}_{int} + \mathbf{f}_{ext}$) for a nonlinear finite element solver. For the sake of your own good, do not look up how much such a software costs on the market. You'd think that we are done, we've just aquired the nice jello effect, show me the C++, please.

Well we definitely have the hardest part defined. However, a key piece is missing: *inertia*! We can integrate through time, but this equilibrium only remains valid if the loads are applied *slowly*. If in actuality the loads are *not* applied slowly, but they're applied rapidly, *inertia forces* need to be considered; i.e., a truly *dynamic problem* needs to be solved.

3.3.1 Equilibrium of a Dynamic Process

According to *'Newton's Second Law'*, we can calculate the inertial force of a particle from $\mathbf{f} = m\mathbf{a}$, where $\mathbf{a}$ is the acceleration vector of the particle. We usually introduce this idea to the finite element method by constructing a mass matrix $\mathbf{M}$ for each element. Then, the inertial forces are calculated as $\mathbf{M}\ddot{\mathbf{u}}$ where $\ddot{\mathbf{u}} = \mathbf{a}$ lists the nodal point accelerations. The element mass matrices are accumulated in the same manner as the element stiffness matrices in the global mass matrix; and the equilibrium equations become

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}_{\text{ext}}. \tag{3.26}$$

The element mass matrix is usually computed by lumping the element's physical mass m to the diagonal, such that

$$\mathbf{M} = m \cdot \mathbf{I}_{n \times n}, \tag{3.27}$$

where n is the number of the element's degree of freedom.

In a real, dynamic system, it is observed that some energy is dissipated during motion. This behaviour is usually taken into account by introducing velocity-dependent damping forces. In this way, the equilibrium equations are further expanded to

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}_{\text{ext}}, \tag{3.28}$$

where $\mathbf{C}$ is the damping matrix of the structure. In practice, it is difficult, if not impossible to determine the element damping parameters for general finite element assemblages. Due to this, the matrix $\mathbf{C}$ in general is *not* assembled from element damping matrices but is constructed using the mass matrix and stiffness matrix of the complete element assemblage together, such that

$$\mathbf{M}\ddot{\mathbf{u}} + (\alpha\mathbf{M} + \beta\mathbf{K})\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}_{\text{ext}}. \tag{3.29}$$

This kind of damping is called *Rayleigh damping* in the literature; and α and β are the damping parameters.

3.3.2 Time Integration

Mathematically, Eq. 3.29 represents a system of linear differential equations of second order and, in principle, the solution to the equations can be obtained by standard procedures for the solution of differential equations with constant coefficients. However, this is just stupid, and not even feasible when the order of the matrices is large.

We have to take advantage of the special characteristics of the coefficient matrices $\mathbf{K}$, $\mathbf{C}$, and $\mathbf{M}$! Such methods are called *time stepping* or *time integration* schemes, and they can be divided into two distinct groups: *explicit* and *implicit* methods.

Explicit Time Integration

Explicit methods calculate the state of a system at a later time from the state of the system at the current time. For example, take a look at the explicit *forward* Euler method:

$$\begin{bmatrix} \mathbf{u} \\ \dot{\mathbf{u}} \end{bmatrix} = h \begin{bmatrix} \dot{\mathbf{x}}_0 \\ \mathbf{M}^{-1}\mathbf{f}_0 \end{bmatrix}. \tag{3.30}$$

Here $\dot{\mathbf{x}}_0$ is the velocity vector of the current timestep, $\mathbf{f}_0 = \mathbf{f}(\mathbf{x}_0, \dot{\mathbf{x}}_0)$, and h is the stepsize.

As you can see, the stiffness matrix, $\mathbf{K}$ is *not* featured in this equation. This makes the implementation of such methods much-much easier than implicit methods, which do require the calculation of $\mathbf{K}$.

However, there is a big catch! Explicit methods require very small timesteps in order to stay stable – or in other words, not to explode. Sometimes timesteps can get so small that the simulation doesn't even move anywhere. Such big timesteps are just not feasible in an interactive framework, so most of the time implicit methods are used, which allows us to use much bigger timesteps.

Implicit Integration

Implicit methods find a solution by solving an equation involving both the current and the later state of the system. They were popularized by Baraff and Witkin by their 98 paper on cloth simulation [2].

They used the implicit *backward* Euler method. Generally, in implicit time integration, $\mathbf{u}$ and $\dot{\mathbf{u}}$ are approximated as

$$\begin{bmatrix} \mathbf{u} \\ \dot{\mathbf{u}} \end{bmatrix} = h \begin{bmatrix} \dot{\mathbf{x}}_0 + \dot{\mathbf{u}} \\ \mathbf{M}^{-1}\mathbf{f}(\mathbf{x}_0 + \mathbf{u}, \dot{\mathbf{x}}_0 + \dot{\mathbf{u}}) \end{bmatrix}. \tag{3.31}$$

The forward method requires only an evaluation of the function $\mathbf{f}$, while the backward method requires that we solve for values of $\mathbf{u}$ and $\dot{\mathbf{u}}$ that satisfy equation Eq. 3.31. Let's do a first order Taylor series expansion on $\mathbf{f}$, which yields

$$\mathbf{f}(\mathbf{x}_0 + \mathbf{u}, \dot{\mathbf{x}}_0 + \dot{\mathbf{u}}) = \mathbf{f}_0 + \frac{\partial \mathbf{f}}{\partial \mathbf{x}}\mathbf{u} + \frac{\partial \mathbf{f}}{\partial \dot{\mathbf{u}}}\dot{\mathbf{u}}. \tag{3.32}$$

Plugging this approximation back to Eq. 3.31 results

$$\begin{bmatrix} \mathbf{u} \\ \dot{\mathbf{u}} \end{bmatrix} = h \begin{bmatrix} \dot{\mathbf{x}}_0 + \dot{\mathbf{u}} \\ \mathbf{M}^{-1}(\mathbf{f}_0 + \frac{\partial \mathbf{f}}{\partial \mathbf{x}}\mathbf{u} + \frac{\partial \mathbf{f}}{\partial \dot{\mathbf{u}}}\dot{\mathbf{u}}) \end{bmatrix}. \tag{3.33}$$

Since $\mathbf{u} = h(\dot{\mathbf{x}} + \dot{\mathbf{u}})$ we have

$$\dot{\mathbf{u}} = h\mathbf{M}^{-1}\left[\mathbf{f}_0 + \frac{\partial \mathbf{f}}{\partial \mathbf{x}}h(\dot{\mathbf{x}} + \dot{\mathbf{u}}) + \frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}}\dot{\mathbf{u}}\right], \tag{3.34}$$

which can then be conveniently regrouped to its final form:

$$\boxed{\left[\mathbf{M} - h\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}} - h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]\dot{\mathbf{u}} = h\mathbf{f} + h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\dot{\mathbf{x}}.} \tag{3.35}$$

Or, you can use the version with $\mathbf{C}$ and $\mathbf{K}$, instead of $\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}}$ and $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$ respectively as

$$\left[\mathbf{M} - h\mathbf{C} - h^2\mathbf{K}\right]\dot{\mathbf{u}} = h\mathbf{f} + h^2\mathbf{K}\dot{\mathbf{x}}; \tag{3.36}$$

altough I think it's much easier to pick up girls in a bar with a partial derivative.

3.4 FEM: Beyond Deformation Simulation

Some interesting stuff in the end: FEM is very popular in geometry processing. Let's look at some examples!

3.4.1 Surface Modelling

The first example is a pretty straightforward one. Imagine the following scenario: you are a 3D designer, and have some arbitrary mesh like leftmost one on Fig. 3.7. If you move e.g. the yellow point around, while the red ones should remain fixed, you probably expect *intuitively*, that the mesh's other vertices are going to move around in the manner it's shown on Fig. 3.7.

How do you formulate this? With FEM, of course! This problem is a regular FEM problem, but instead of telling the system what the loads are, we'll tell it where a set of vertices should be – there is a neat trick for formulating this as well, presented in Sec. 7.3. The As-Rigid-As-Possible (ARAP) surface modelling method [27] presents nothing but a nonlinear FEM based solver, however, they defined their own new strain energy function:

$$\Psi_{\text{ARAP}} = \frac{\mu}{2}\|\mathbf{F} - \mathbf{R}\|_F^2. \tag{3.37}$$

Here $\|\cdot\|_F^2$ is the Frobenius norm (Sec. 4.4.1) turning a matrix (tensor) into a scalar. $\mathbf{F}$ is the deformation gradient of course, while $\mathbf{R}$ is the rotational part of $\mathbf{F}$ – arising from the polar decomposition of $\mathbf{F}$. (Sec. 4.1.4)

This energy function can actually be used in deformation simulation as well, and has some nice properties, that we are going to discuss in Chapter 5 and 6.

3.4.2 Geometry Optimization

This is a bit more meta: meshes for FEM simulations are made with... FEM! Crazy right? Turns out that the finite element formulation is a pretty nice measure for the *'niceness'* of meshes: again, intuitively you'd expect a volumetric mesh's elements to be evenly distributed, each element having kind of the same, uniform edge length and volume.

The FEM-based approach for this problem does nothing but applies FEM: they start with a basic (random) Delaunay-triangulation, then consistently minimize a global energy function over the domain by relocating the vertices at each step. In the end they end up with a mesh where the energy is evenly distributed.

Aside from its use for FEM meshes [1], they use it for surface parametrization as well (Fig. 3.8). This is a pretty big thing, because the reparametrization of surfaces is still done by hand, consuming hundreds of hours of expensive man-power.

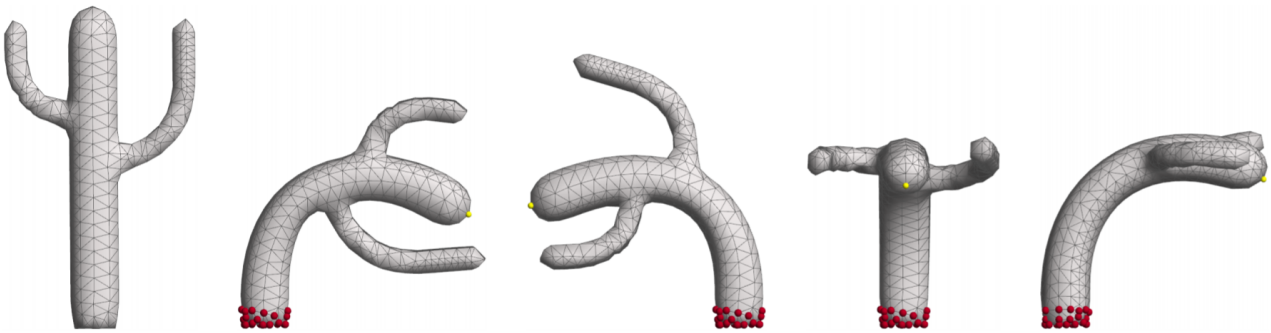


Figure 3.7: As-Rigid-As-Possible surface modelling [27].

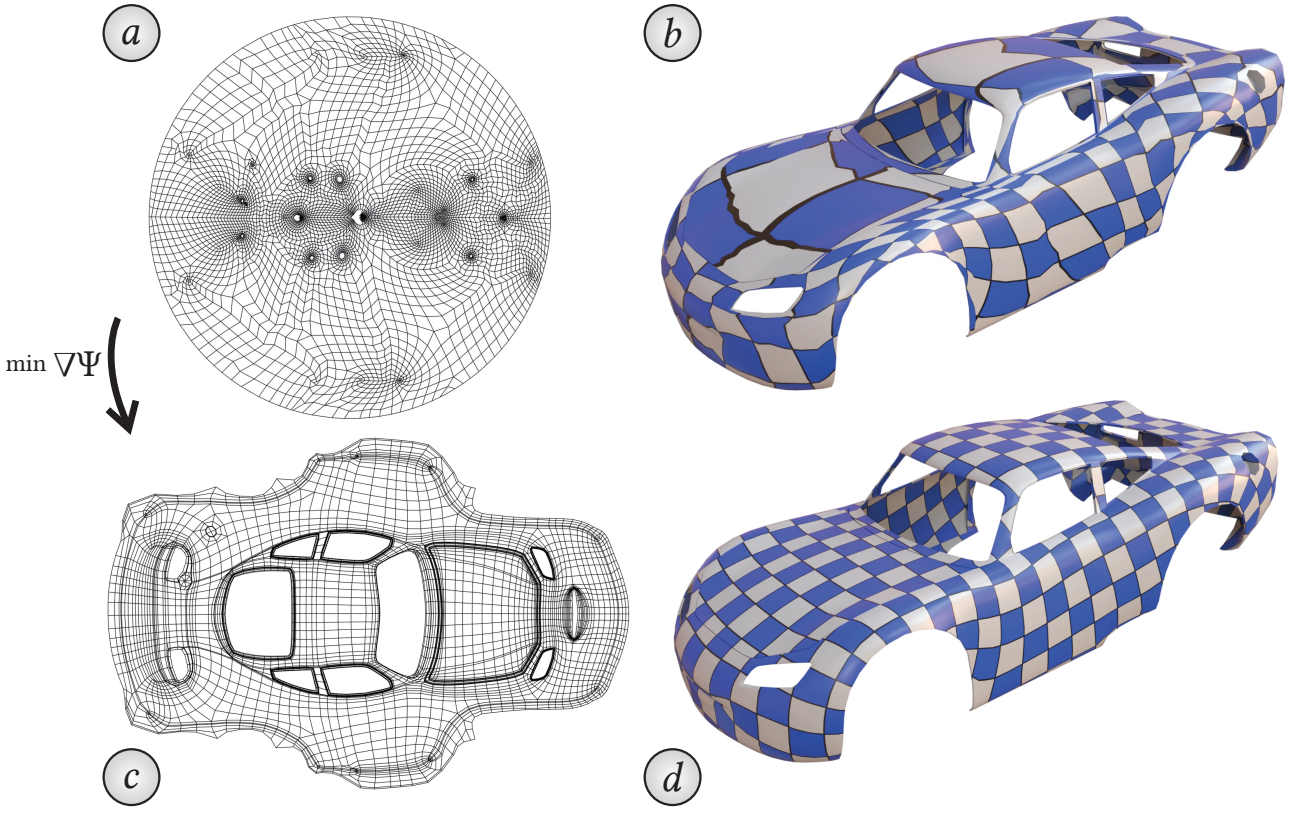


Figure 3.8: Optimizing surface parametrization: Initial surface parametrization *(a)* results in poor utilization of the per-pixel color data *(b)* a.k.a. texture of the surface. Optimizing for consistent *'deformation energy'* Ψ achieves the desired parametrization automatically *(c & d)* [25].

Chapter 4

Fundamentals of Continuum Mechanics

Continuum mechanics is a branch of mechanics that deals with the mechanical behavior of materials modeled as a continuous mass rather than as discrete particles.

The initial objective of continuum mechanics is to provide a concise, coherent mathematical description of the deformation and motion that an elastic body has sustained. Then, we can use these measures to quantify stuff about the deformation. For example, both *Piola-Kirchhoff stress* $\mathbf{P}$ or the *strain energy* Ψ are computed from the kinematic measures; and they are essential in the finite element formulation as well.

If you really want to dig deep into continuum mechanics, I highly recommend the two classics on the subject: the books by Bonet – Wood [6] and Holzapfel [9].

4.1 Kinematics

Let's begin our journey into continuum mechanics by exploring the set of kinematic measures we are going to use.

4.1.1 Motion

Fig. 4.1 shows the general motion of the deformable body. The body is an assemblage of particles labeled by the coordinates $\mathbf{x}$ with respect to the Cartesian basis $\mathbf{e}_i$, at their initial positions at time $t = 0$. Generally, the current positions of these particles are located, at time = t, by the coordinates $\overline{\mathbf{x}}$ with respect to an alternative Cartesian basis $\overline{\mathbf{e}_i}$. In the remainder of this document, $\mathbf{e}_i$ and $\overline{\mathbf{e}_i}$ will be taken to be coincident. Alternatively these *initial* and *current* configurations are referred as *material* or *Lagrangian* and *spatial* or *Eulerian* descriptions in the literature.

With the particle positions precisely defined, we can describe the motion mathematically as a mapping ϕ between initial and current particle positions as

$$\overline{\mathbf{x}} = \phi(\mathbf{x}, t). \tag{4.1}$$

For a fixed value of t the above equations represent a mapping between the undeformed and deformed bodies. Additionally, for a fixed particle $\mathbf{x}$, Eq. 4.1 describes the motion or trajectory of this particle as a function of time.

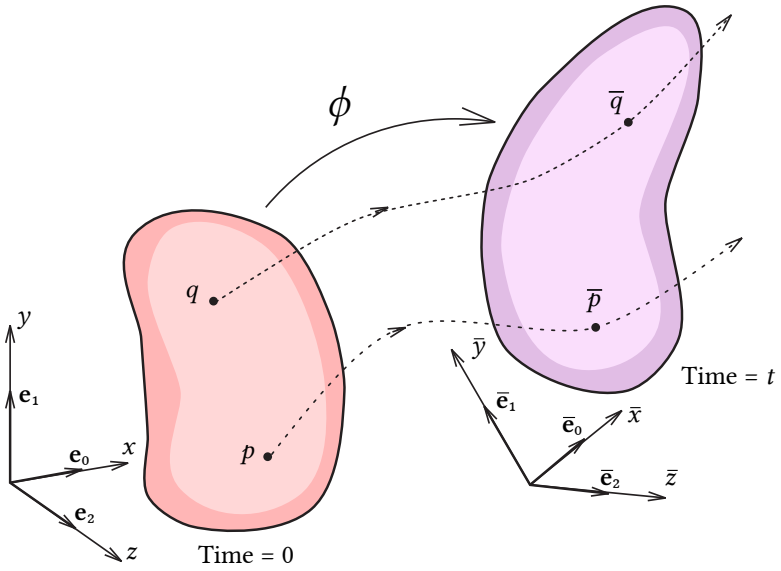


Figure 4.1: General motion of the body

It is important to note here that I just departed from the regular notation in continuum mechanics: the initial *(material)* configuration is usually denoted by uppercase letters – e.g. $\mathbf{X}$ and $\mathbf{E}_I$ – while lowercase letters mark the current *(spatial)* configuration: e.g. $\mathbf{x}$ and $\mathbf{e}_i$ respectively. I ditched this notation and used the *overline* operator – $\overline{\mathbf{x}}$ and $\overline{\mathbf{e}}$ – to denote the current *(spatial)* configuration as seen above. It has a practical reason: in the subsequent chapters, a significant amount of linear algebra and tensor trickery will be present, so it's easier to follow the train of thought with lowercase letters denoting vectors ($\mathbf{a}$) and uppercase ones matrices ($\mathbf{A}$).

4.1.2 Deformation Gradient

While ϕ characterizes the general motion of the body, there is a measure, which precisely quantifies the deformation – that is, all the *rotation* and *scaling* – at each quadrature point: it's the deformation gradient, denoted by $\mathbf{F}$, which I briefly introduced it in Sec. 3.2.2. It is among the important quantities of deformable simulation, we calculate *everything* from $\mathbf{F}$: it is involved in all equations *relating quantities before deformation to corresponding quantities after (or during) deformation.* The deformation gradient tensor enables the relative *spatial* position of a particle after deformation to be described in terms of its relative *material* position before deformation.

Let's derive it! In order to do so, consider the infinitesimal material line elements $d\mathbf{x}$ and $d\,\overline{\mathbf{x}}$ originating from material particles p and $\overline{p}$ according to Fig. 4.2. After deformation, the material particles p and $d\mathbf{x}$ in the initial configuration can be described in the current configuration as

$$\overline{\mathbf{x}} + d\,\overline{\mathbf{x}} = \phi(\mathbf{x} + d\mathbf{x}, t). \tag{4.2}$$

This can be further expanded to

$$\overline{\mathbf{x}} + d\,\overline{\mathbf{x}} = \phi(\mathbf{x}, t) + \frac{\partial \phi(\mathbf{x}, t)}{\partial \mathbf{x}} d\mathbf{x}. \tag{4.3}$$

As $\overline{\mathbf{x}} = \phi(\mathbf{x}, t)$, from Eq. 4.3 we have

$$d\,\overline{\mathbf{x}} = \frac{\partial \phi(\mathbf{x}, t)}{\partial \mathbf{x}} d\mathbf{x}. \tag{4.4}$$

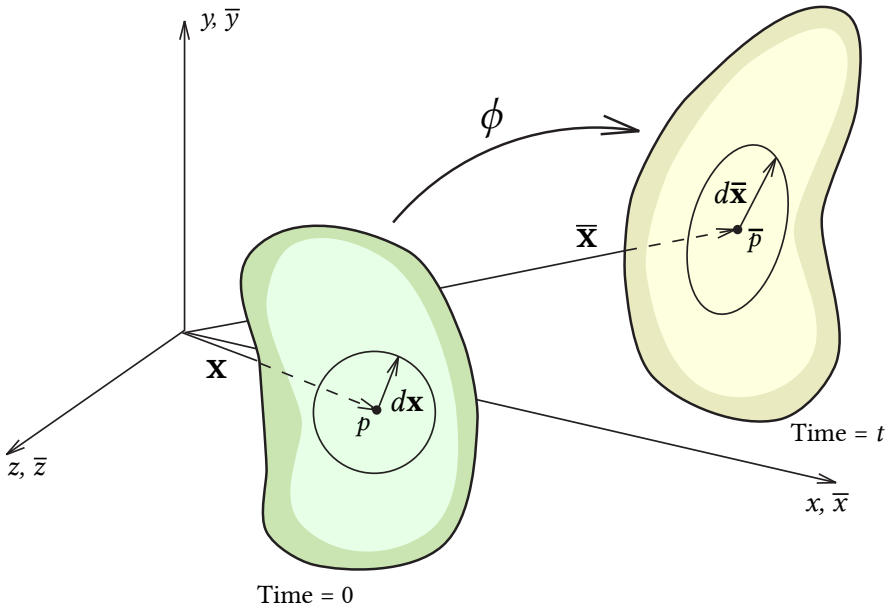


Figure 4.2: The Deformation Gradient

The thing on the right hand side is the deformation gradient:

$$\boxed{\mathbf{F} = \frac{\partial \phi}{\partial \mathbf{x}}.} \tag{4.5}$$

It's pretty much just the derivative of the motion:

$$\mathbf{F} = \begin{bmatrix} \partial \bar{x}/\partial x & \partial \bar{x}/\partial y & \partial \bar{x}/\partial z \\ \partial \bar{y}/\partial x & \partial \bar{y}/\partial y & \partial \bar{y}/\partial z \\ \partial \bar{z}/\partial x & \partial \bar{z}/\partial y & \partial \bar{z}/\partial z \end{bmatrix}. \tag{4.6}$$

Alternatively, you can write

$$d\bar{\mathbf{x}} = \mathbf{F} d\mathbf{x}, \tag{4.7}$$

which I think shows pretty well how **F** transforms vectors in the initial configuration into vectors in the current configuration.

A very important property coming up: changing the configuration, i.e. translating our material particle by an arbitrary vector, **t** *does nothing to a deformation gradient*:

$$\bar{\mathbf{x}} = \phi(\mathbf{x}) = \mathbf{x} + \mathbf{t} \quad \rightarrow \quad \mathbf{F} = \frac{\partial \phi(\mathbf{x})}{\partial \mathbf{x}} = \mathbf{I} \tag{4.8}$$

t just burned away! It is said that **F** is an *objective measure*. No matter how much *rigid-body* translation you apply to an element, it doesn't do anything with **F**. See [9] Chapter 5 for more information about *objectivity*.

Hopefully I was able to grasp the essence of the deformation gradient. Right now, it is not important *exactly* how you would compute the quantity – it has its own section. (Sec. 7.1) So for the time being, just try to *feel* what **F** means.

4.1.3 Strain

To simplify analysises, the *concept* of strain tensors are introduced. It is nothing but another geometric representation to measure deformation. The right Cauchy-Green deformation tensor $\mathbf{C}$ is defined as

$$\mathbf{C} = \mathbf{F}^T\mathbf{F}, \tag{4.9}$$

while the material Green-Lagrange strain tensor $\mathbf{E}$ is calculated from

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}) = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I}). \tag{4.10}$$

4.1.4 Polar Decomposition

The deformation gradient $\mathbf{F}$ transforms any vector in the material coordinate system to one in the spatial coordinate system. We also stated that rigid-body translations are *not* included in $\mathbf{F}$, so it only encodes *all* the *rotation* and *stretching* the material particle has sustained. Now the thing is that you can actually factor out the separate rotational $\mathbf{R}$ and stretching component $\mathbf{S}$ from $\mathbf{F}$, while

$$\mathbf{F} = \mathbf{RS}. \tag{4.11}$$

Here, $\mathbf{S}$ denotes the right stretch tensor. Note that in the continuum mechanics literature, $\mathbf{S}$ is usually denoted by $\mathbf{U}$; while there's a left stretch tensor $\mathbf{V}$ as well, coming from the Eulerian factorization of $\mathbf{F} = \mathbf{VR}$. I used $\mathbf{S}$ instead (following [15]), because $\mathbf{U}$ (and also $\mathbf{V}$) is reserved for the result of the singular value decomposition.
Remember the As-Rigid-As-Possible (ARAP) energy from Sec. 3.4.2? It was

$$\Psi_{\text{ARAP}} = \frac{\mu}{2}\|\mathbf{F} - \mathbf{R}\|_F^2, \tag{4.12}$$

where $\mathbf{R}$ is of course the rotational part of $\mathbf{F}$. We are going to use this energy a lot, so we need an efficient approach to factorize $\mathbf{R}$ from $\mathbf{F}$.

Compute Polar Decomposition from SVD

One method to factorize $\mathbf{F}$ into $\mathbf{R}$ and $\mathbf{S}$ is by taking the *singular value decomposition (SVD)* of it. SVD is a factorization of some matrix $\mathbf{A}$ to its constituent parts, such that

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T. \tag{4.13}$$

$\mathbf{U}$ and $\mathbf{V}$ are the left- and right singular vectors, representing rotations, while Σ is a scaling by the singular values. See Fig. 4.3 for reference.
A cool thing about this SVD is that if you apply on $\mathbf{F}$:

$$\mathbf{F} = \hat{\mathbf{U}}\hat{\Sigma}\hat{\mathbf{V}}^T, \tag{4.14}$$

you can pretty easily get $\mathbf{S}$ and $\mathbf{R}$ as

$$\hat{\mathbf{R}} = \hat{\mathbf{U}}\hat{\mathbf{V}}^T, \tag{4.15}$$

$$\hat{\mathbf{S}} = \hat{\mathbf{V}}\hat{\Sigma}\hat{\mathbf{V}}^T. \tag{4.16}$$

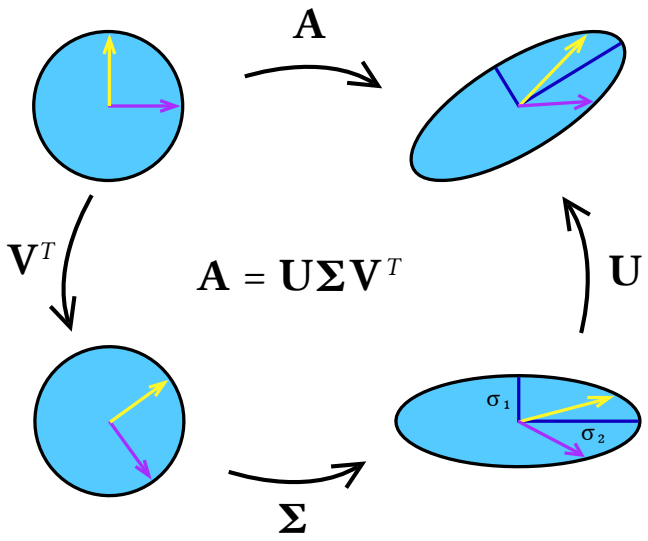


Figure 4.3: Singular value decomposition of some matrix **A**.

Okay but we need **S** and **R**, not $\hat{\mathbf{S}}$ and $\hat{\mathbf{R}}$, what's up with all the hatting?

There's a small caveat as – following Teran et al. [12] – we need a *rotationally variant* SVD. The basic SVD factorization only guarantees that **R** is a unitary matrix – that is $\mathbf{R}^T\mathbf{R} = \mathbf{I}$. This means that there could be a reflection lurking somewhere in **R**, whereas we want **R** to be a pure rotation. In our case, if a reflection has to lurk somewhere, we would prefer that it does so in **S**.

There's a pretty neat way to pull this off by Sorkine-Hornung and Rabinovich [28]. It is presented in [15], Appendix F. Of course, you will end up with the unhatted values:

$$\mathbf{R} = \mathbf{U}\mathbf{V}^T, \tag{4.17}$$

$$\mathbf{S} = \mathbf{V}\mathbf{\Sigma}\mathbf{V}^T. \tag{4.18}$$

4.1.5 Volume change

Another very important kinematic measure is the volume change of an element, denoted by J, which can be easily computed from

$$J = \det \mathbf{F}. \tag{4.19}$$

4.2 The Concept of Stress

In the previous section some kinematic aspects of the motion and deformation of the continuum body were discussed. Motion and deformation give rise to interactions between the neighboring particles in the interior part of the body. One consequence of these interactions is stress, which has the physical dimension *force per unit area.*

(Yet again) consider a general deformable body under load as in Fig. 4.4. Let's cut the body by a plane with a surface normal $\mathbf{n}$ at any given point $\mathbf{x} \in \Omega$, resulting two regions, R_1 and R_2. In order to develop the *concept of stress*, we should study the action of forces, applied by one region (R_1) to the remaining part of the body (R_2).

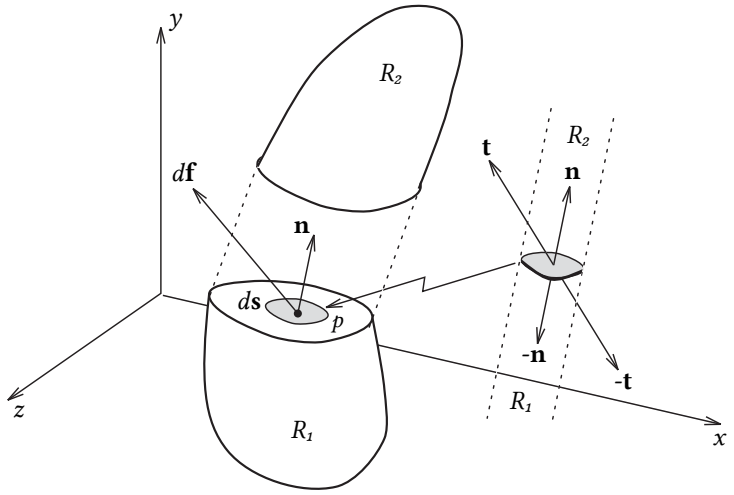


Figure 4.4: The concept of stress in the *material* coordinate system.

For this purpose, let's examine some infinitesimal area ds on the cutting-plane. Since forces are transmitted across the internal plane surface, we can define a *resultant* force acting on the surface element as $d\mathbf{f}$. According to Fig. 4.4 for every surface element

$$d\mathbf{f} = \bar{\mathbf{t}} d\bar{s} = \mathbf{t} ds, \tag{4.20}$$

where

$$\bar{\mathbf{t}} = \bar{\mathbf{t}}(\bar{\mathbf{x}}, t, \bar{\mathbf{n}}) \tag{4.21}$$

represents the *Cauchy traction vector* – force measured per unit surface area defined in the *current* configuration – exerted on $d\bar{s}$ with outward normal $\bar{\mathbf{n}}$. On the other hand,

$$\mathbf{t} = \mathbf{t}(\mathbf{x}, t, \mathbf{n}) \tag{4.22}$$

represent the *first Piola-Kirchhoff traction vector* – force measured per unit surface area defined in the *reference* configuration. Again, both traction vectors measure how much one side is pushing on the other side in case of some specific loading condition.

Cauchy's stress theorem states, that unique second-order tensor fields – σ and $\mathbf{P}$ – exist, such that

$$\begin{aligned} \bar{\mathbf{t}}(\bar{\mathbf{x}}, t, \bar{\mathbf{n}}) &= \sigma(\bar{\mathbf{x}}, t)\bar{\mathbf{n}}, \\ \mathbf{t}(\mathbf{x}, t, \mathbf{n}) &= \mathbf{P}(\mathbf{x}, t)\mathbf{n}, \end{aligned} \tag{4.23}$$

where σ denotes the *spatial* tensor field called *Cauchy stress tensor*, while $\mathbf{P}$ characterizes a tensor field called *first Piola-Kirchhoff stress tensor* in the *reference* configuration.

Relation 4.23 is one of the most important axioms of continuum mechanics. It basically states that if a traction vector such as $\mathbf{t}$ or $\bar{\mathbf{t}}$ depend on the outward unit normals $\mathbf{n}$ or $\bar{\mathbf{n}}$, then they must be *linear in* $\mathbf{t}$ *or* $\bar{\mathbf{t}}$, respectively.
Furthermore, an immediate consequence of Eq. 4.23 is that

$$\mathbf{t}(\mathbf{x}, t, \mathbf{n}) = -\mathbf{t}(\mathbf{x}, t, -\mathbf{n}), \tag{4.24}$$

for all unit vectors $\mathbf{n}$. This is known as *Newton's third law of action and reaction* and it applies in the reference configuration as well (omitted here).

4.3 Balance Laws

We've gotten a pretty concise description of motion, and introduced the concept of stress, which are two important building blocks when we try to model some *'physically based'* deformable phenomena. However, there are two key pieces missing. Actually, we've already talked about one of them: in Sec. 3.2.2, we briefly have introduced the concept of total potential energy, which allowed us to completely characterize the response of the physical phenomena of a strain energy-based deformable model, i.e.

$$\Pi_{int} + \Pi_{ext} = \text{const}, \tag{4.25}$$

$$\Pi_{int} = \int_{\Omega_0} \Psi(\mathbf{F}) dV. \tag{4.26}$$

For our purposes, we don't need to worry too much about where this idea is derived from. If you are interested, I highly recommend you going through Holzapfel's derivation in [9], Chapter 4. It can be derived precisely from the conservation of mass, and the balance of linear and angular momentum (a.k.a. Newton's first and second law).

4.4 The Hyperelastic Constitutive Model

It's only a single Lego-block that is missing at this point: what is that energy function Ψ? The thing we haven't talked about yet is the material the body in discussion is made of. All the things described here, the kinematics, stresses, balance principles, hold for any continuum body. The energy function Ψ is what distinguishes whether if we talk about steel or a piece of well chewed gum.

In this text, we are going to use a special energy function, exploiting that we are considering a conservative system: we are going to use the hyperelastic material – or more 'scientifically' *constitutive* – model.

The hyperelastic constitutive model is a phenomenological approach modeling perfectly elastic material. In this context perfectly elastic means that no matter how much I abuse a piece of rubber, after the loads are removed, the body will recover to its original state. This means that we can characterize hyperelastic models exclusively with the deformation gradient, so the energy function, Ψ, becomes the strain energy function, $\Psi(\mathbf{F})$.

$\Psi(\mathbf{F})$ assigns the deformation score to a specific $\mathbf{F}$, which is a scalar, making $\Psi(\mathbf{F})$ a scalar valued tensor function. Then as we have already seen it in Eq. 3.23, we'll need to take the Jacobian and Hessian of it in order to timestep our Newton-solver. It surely doesn't sound as fun as it's going to be. Chapter 5 will be all about that.

If you want to be a constitutive god, I have to point you again to Holzapfel's masterpiece [9], but this time to Chapter 6.

There are two very important properties of the strain energy function in case of hyperelastic material models, which we are going to exploit in the following chapters.

First, strain energy vanishes in the reference configuration, or in other words, if there is no motion: $\mathbf{F} = \mathbf{I}$. That is

$$\Psi(\mathbf{I}) = 0. \tag{4.27}$$

Second, if $\mathbf{F} = \mathbf{R}$, that is, the motion is some *pure rigid-body rotation*

$$\Psi(\mathbf{R}) = 0. \tag{4.28}$$

We will elaborate on this a lot in Sec. 5.5.

4.4.1 What Does an Energy Function Look Like?

$\Psi(\mathbf{F})$ is a scalar valued tensor function. You plug in a tensor, $\mathbf{F}$, and you get a scalar back. But how do you boil a matrix down to a number exactly?

One way to do that is to define energy functions as the squared Frobenius norm. You might not have heard about it, so let me just define it for you.

The Squared Frobenius Norm

Consider a matrix

$$\mathbf{A} = \begin{bmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{bmatrix}, \tag{4.29}$$

then the squared Frobenius norm of matrix $\mathbf{A}$, denoted by $\|\mathbf{A}\|_F^2$ is

$$\boxed{\|\mathbf{A}\|_F^2 = \sum_{i=0}^{2}\sum_{j=0}^{2} a_{ij}^2.} \tag{4.30}$$

So it's just summing up all the squared entries of matrix $\mathbf{A}$.

Why would you do such a thing? It feels a bit... arbitrary, isn't it? It surely felt as such for me, when I first come across these norms. Doesn't anybody care which row and column these entries came from? Surely their order in the matrix should count for something?

Well the point is that first: there isn't much else you can do when you want to distill the *'essence'* of some vector or a matrix into a single number. You can take the square root of this, or if it's a matrix, maybe you can calculate the trace, but none of these do something fundamentally differently than the squared Frobenius norm.

Second of all – and more importantly – it gets the job done. And I'm – hopefully going to be soon – an engineer so it's all I care about at this point. For me, it actually got the job done so well, that I started using norms a lot. E.g. if you program any linear algebra, it's a pretty neat way to *'debug'* huge matrices and vectors.

An Energy Function

We've got a nice way to boil down a matrix to a scalar. Let's just use it and have a look at an energy function. You get the stretching part of the Saint-Venant Kirchhoff energy if you take the squared Frobenius norm of the Green strain from Eq. 4.10:

$$\Psi_{\text{StVK,stretch}} = \|\mathbf{E}\|_F^2 = \frac{1}{4}\|\mathbf{F}^T\mathbf{F} - \mathbf{I}\|_F^2. \tag{4.31}$$

In the next chapter we are going to use this form a lot. Buckle up, because we are about to take a deep in the inner workings of energy functions, and its Jacobians and Hessians.

Chapter 5

Jacobians and Hessians

Either you go down the quasistatic way

$$\mathbf{K}\mathbf{u} = \mathbf{f}_{int} - \mathbf{f}_{ext}, \tag{5.1}$$

$$\mathbf{f}_{int} = -v\frac{\partial \Psi}{\partial \mathbf{x}}, \qquad \mathbf{K} = -v\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = -v\frac{\partial^2 \Psi}{\partial \mathbf{x}^2}, \tag{5.2}$$

or the backward Euler way

$$\left[\mathbf{M} - h\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}} - h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]\dot{\mathbf{u}} = h\mathbf{f} + h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\dot{\mathbf{x}}, \tag{5.3}$$

you need to compute both the *Jacobian* $\frac{\partial \Psi}{\partial \mathbf{x}}$ and the *Hessian* $\frac{\partial^2 \Psi}{\partial \mathbf{x}^2}$ of the strain energy function $\Psi(\mathbf{F})$. But how would you do that? $\Psi(\mathbf{F})$ is a scalar valued tensor function; how do you take its derivative in terms of $\mathbf{x}$, which is a vector? And what is a tensor anyways? Don't worry, we are going to go through the $\frac{\partial \Psi}{\partial \mathbf{x}}$ and $\frac{\partial^2 \Psi}{\partial \mathbf{x}^2}$ computation extensively, following Kim in [15].

Let's take one step at a time and try to compute $\mathbf{f}_{int}$! First we need to stack the vertices of our element of choice into a big vector – e.g. for a 2D triangle this vector is

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} x_0 \\ y_0 \\ x_1 \\ y_1 \\ x_2 \\ y_2 \end{bmatrix}, \tag{5.4}$$

then take the gradient of it:

$$\mathbf{f} = -a\frac{\partial \Psi}{\partial \mathbf{x}}. \tag{5.5}$$

Here a is the area of the original triangle at rest. As you can see, in 2D we multiply with a instead of v.

To be able to deal with this problem, we need to apply the good ole' chain rule that separates $\frac{\partial \Psi}{\partial \mathbf{x}}$ into two components:

$$\frac{\partial \Psi}{\partial \mathbf{x}} = \frac{\partial \Psi}{\partial \mathbf{F}} : \frac{\partial \mathbf{F}}{\partial \mathbf{x}}. \tag{5.6}$$

Not much friendlier looking, is it? And there are several hidden *'gotcha'*s as well, what we need to address here before we progress to calculate the force jacobians $\frac{\partial^2 \Psi}{\partial \mathbf{x}^2}$.

5.1 Higher-Order Tensor Manipulations

The first term in Eq. 5.6 is relatively easy. $\Psi \in \mathfrak{R}$ and $\mathbf{F} \in \mathfrak{R}^{3\times3}$, so the derivative is just a matrix:

$$\frac{\partial \Psi}{\partial \mathbf{F}} = \begin{bmatrix} \frac{\partial \Psi}{\partial f_{00}} & \frac{\partial \Psi}{\partial f_{10}} & \frac{\partial \Psi}{\partial f_{20}} \\ \frac{\partial \Psi}{\partial f_{01}} & \frac{\partial \Psi}{\partial f_{11}} & \frac{\partial \Psi}{\partial f_{21}} \\ \frac{\partial \Psi}{\partial f_{02}} & \frac{\partial \Psi}{\partial f_{12}} & \frac{\partial \Psi}{\partial f_{22}} \end{bmatrix}. \tag{5.7}$$

Here f_{ij} are the scalar entries of $\mathbf{F}$. The result clearly is a 3×3 matrix, also known as a *2^{nd}-order tensor.*

5.1.1 Mental Representation of Higher-Order Tensors

The confusion begins when we try to compute $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$. Since $\mathbf{F} \in \mathfrak{R}^{3\times3}$ is a matrix and $\mathbf{x} \in \mathfrak{R}^{12}$ (or $\mathfrak{R}^{6}$ in 2D). The first entry of $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ would look like then

$$\frac{\partial \mathbf{F}}{\partial x_0} = \begin{bmatrix} \frac{\partial f_{00}}{\partial x_0} & \frac{\partial f_{10}}{\partial x_0} & \frac{\partial f_{20}}{\partial x_0} \\ \frac{\partial f_{01}}{\partial x_0} & \frac{\partial f_{11}}{\partial x_0} & \frac{\partial f_{21}}{\partial x_0} \\ \frac{\partial f_{02}}{\partial x_0} & \frac{\partial f_{12}}{\partial x_0} & \frac{\partial f_{22}}{\partial x_0} \end{bmatrix}. \tag{5.8}$$

Already, the result is a matrix. Taking the derivates with respect to the next entries of $\mathbf{x}$, we will have a pile of matrices, 12 of them actually. There are many methods for dealing with such structures; e.g. you might come across the so called *Einstein* or *indical notation* during your continuum mechanics studies.

The dimenson of the derivative $\frac{\partial \mathbf{F}}{\partial \mathbf{x}} \in \mathfrak{R}^{3\times3\times12}$, where the third dimension is the big giveaway that we're looking at a 3rd-order tensor. Many textbooks prefer to think of these as a cube of matrices, but for our purposes a *vector of matrices* is the most straightforward mental image – see Fig. 5.1 for visualisation.

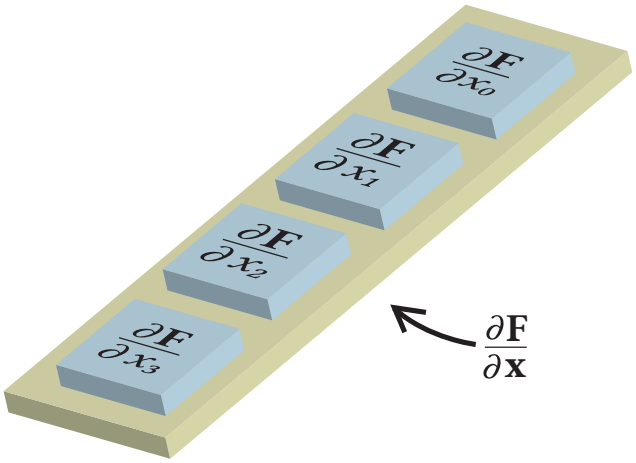


Figure 5.1: Thinking about 3rd-order tensors as a vector of matrices.

That is, some 3rd-order tensor $\mathbb{A}$ looks like

$$\mathbb{A} = \begin{bmatrix} \begin{bmatrix} a & c \\ b & d \end{bmatrix} \\ \begin{bmatrix} e & g \\ f & h \end{bmatrix} \\ \begin{bmatrix} i & k \\ j & l \end{bmatrix} \end{bmatrix} = \begin{bmatrix} [\mathbf{A}] \\ [\mathbf{B}] \\ [\mathbf{C}] \end{bmatrix}. \tag{5.9}$$

5.1.2 Multiplication With Higher-Order Tensors

After dealing with the *'mental image'* of higher-order tensors, all that's left to discuss from $\frac{\partial \Psi}{\partial \mathbf{F}} : \frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ is the funky ':' sign. It denotes the *double-contraction* operation. *Contracting* two *matrices* together would be like

$$\mathbf{A} : \mathbf{B} = \begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} \begin{bmatrix} b_0 & b_2 \\ b_1 & b_3 \end{bmatrix} = a_0 b_0 + a_1 b_1 + a_2 b_2 + a_3 b_3. \tag{5.10}$$

Pretty easy! Just sum up the product of each entry (like $\sum a_i b_i$). However, $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ is not a matrix, but a 3rd-order tensor. A 3rd vs. 2nd double-contraction is defined as

$$\mathbb{A} : \mathbf{B} = \begin{bmatrix} \begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} \\ \begin{bmatrix} a_4 & a_6 \\ a_5 & a_7 \end{bmatrix} \\ \begin{bmatrix} a_8 & a_{10} \\ a_9 & a_{11} \end{bmatrix} \end{bmatrix} \begin{bmatrix} b_0 & b_2 \\ b_1 & b_3 \end{bmatrix} = \begin{bmatrix} a_0 b_0 + a_1 b_1 + a_2 b_2 + a_3 b_3 \\ a_4 b_0 + a_5 b_1 + a_6 b_2 + a_7 b_3 \\ a_8 b_0 + a_9 b_1 + a_{10} b_2 + a_{11} b_3 \end{bmatrix}. \tag{5.11}$$

It's not that hard either! It is basically the same operation as with matrices, but we contract the 2nd-order one against each *'submatrix'* of the higher-order tensor. Stacking the results on top of each other yields a good ole' vector.

5.1.3 Vectorization

So far so good, but working with higher-order tensors in high-performance code becomes pretty cumbersome. However, there's a solution, which will make our life much simpler: the act of *vectorization* or simply *flattening* turns any tensor, be it 3rd-order, 4th-order, or 100th-order, back into the familiar 2nd-order matrix form. The vectorized representation was popularized by Pixar in [24].

We introduce the vectorization operator $\text{vec}(\,\cdot\,)$ to convert any matrix to a vector, and any higher-order tensor to a matrix. First up, this is how it converts a matrix to a vector:

$$\text{vec}(\mathbf{A}) = \text{vec}\left(\begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} \right) = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix}. \tag{5.12}$$

The important pattern to notice is that we've *stacked the columns on top of each other.* The flattening convention of a 3rd-order tensor looks like

$$\mathrm{vec}(\mathbb{A}) = \mathrm{vec}\begin{bmatrix} [\mathbf{A}] \\ [\mathbf{B}] \\ [\mathbf{C}] \end{bmatrix} = \begin{bmatrix} \mathrm{vec}(\mathbf{A}) & \mathrm{vec}(\mathbf{B}) & \mathrm{vec}(\mathbf{C}) \end{bmatrix}, \tag{5.13}$$

which expands to

$$\mathrm{vec}\left[\begin{bmatrix}\begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} \\ \begin{bmatrix} a_4 & a_6 \\ a_5 & a_7 \end{bmatrix}\end{bmatrix} \\ \begin{bmatrix} a_8 & a_{10} \\ a_9 & a_{11} \end{bmatrix}\right] = \begin{bmatrix} \mathrm{vec}\begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} & \mathrm{vec}\begin{bmatrix} a_4 & a_6 \\ a_5 & a_7 \end{bmatrix} & \mathrm{vec}\begin{bmatrix} a_8 & a_{10} \\ a_9 & a_{11} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_0 & a_4 & a_8 \\ a_1 & a_5 & a_9 \\ a_2 & a_6 & a_{10} \\ a_3 & a_7 & a_{11} \end{bmatrix}. \tag{5.14}$$

The big advantage of using a vectorized form of tensors is that we can replace the mighty double contraction operation with a conventional matrix multiply, as follows:

$$\mathbb{A} : \mathbf{B} = (\mathrm{vec}\ \mathbb{A})^T \mathrm{vec}\ \mathbf{B}. \tag{5.15}$$

5.2 Computing Forces

With all the tensor stuff in place, we can finally compute some forces. Once again it's calculated from $\mathbf{f} = -v\frac{\partial \Psi}{\partial \mathbf{x}}$, and with the chain rule it becomes

$$\frac{\partial \Psi}{\partial \mathbf{x}} = \frac{\partial \Psi}{\partial \mathbf{F}} : \frac{\partial \mathbf{F}}{\partial \mathbf{x}}. \tag{5.16}$$

The trick is that the 3rd-order tensor, $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ has a static, simple, and energy-independent structure that stays the same through the simulation. It has to be derived and coded only once for each element type. For the time being, let's just assume we have this $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ – as it's actually featured in Sec. 7.1.2.

The other term, $\frac{\partial \Psi}{\partial \mathbf{F}}$ is what we care about! Do you remember the *first Piola-Kirchhoff stress tensor*? I've already introduced it in Sec. 4.2. It is denoted by $\mathbf{P}$, and believe it or not,

$$\frac{\partial \Psi(\mathbf{F})}{\partial \mathbf{F}} = \mathbf{P}(\mathbf{F}). \tag{5.17}$$

Isn't it wonderful? And the best thing is that if you want to use a new energy, all you need to do is to derive a new $\mathbf{P}$ a.k.a. $\frac{\partial \Psi}{\partial \mathbf{F}}$.

If you've got both terms, you can go down the double contraction route as of Eq. 5.16, or use our fancy new vectorization method to compute things purely matrix. The latter approach yields

$$\frac{\partial \Psi}{\partial \mathbf{x}} = \mathrm{vec}\left(\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right)^T \mathrm{vec}\left(\frac{\partial \Psi}{\partial \mathbf{F}}\right). \tag{5.18}$$

5.2.1 Examples

With all this knowledge, computing forces becomes pretty easy! To get the hang of Frobenius norms, let's take a look at some examples on calculating $\mathbf{P}$.

St. Venant-Kirchhoff

The St. Venant-Kirchhoff energy is defined as

$$\Psi_{\text{StVK}} = \mu\|\mathbf{E}\|_F^2 + \frac{\lambda}{2}(\text{tr}\mathbf{E})^2. \tag{5.19}$$

Here, the first member, $\|\mathbf{E}\|_F^2$ is the stretching term, while $(\text{tr}\mathbf{E})^2$ is the volume preservation one. With the constants μ and λ you can tell the model how much relative stretching resistance vs. volume preservation you want.

First let's deal with $\|\mathbf{E}\|_F^2$. Recall from Eq. 4.10 that Green Strain $\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I})$. Plug this in the energy function and expand the Frobenius norm using the identities $\|\mathbf{A}+\mathbf{B}\|_F^2 = \|\mathbf{A}\|_F^2+\|\mathbf{B}\|_F^2-2\text{tr}\mathbf{A}^T\mathbf{B}$ and $\text{tr}(\mathbf{F}^\mathbf{T}\mathbf{F}) = \|\mathbf{F}\|_F^2$ such that

$$\Psi_{\text{StVK,stretch}} = \frac{1}{4}\|\mathbf{F}^T\mathbf{F} - \mathbf{I}\|_F^2 = \frac{1}{4}\|\mathbf{F}^T\mathbf{F}\|_F^2 + \text{tr}\mathbf{I} - 2\|\mathbf{F}\|_F^2. \tag{5.20}$$

tr$\mathbf{I}$ burns away during differentiation, so the $\mathbf{P}$ of the stretching term becomes

$$\begin{aligned}\mathbf{P}_{\text{StVK,stretch}} &= \frac{1}{4}\left(4\mathbf{F}\mathbf{F}^T\mathbf{F} - 4\mathbf{F}\right)\\ &= \mathbf{F}\left(\mathbf{F}^T\mathbf{F} - \mathbf{I}\right)\\ &= \mathbf{F}\mathbf{E}.\end{aligned} \tag{5.21}$$

It's so easy I could even recall this during an exam! The complete StVK is not that hard either:

$$\mathbf{P}_{\text{StVK}} = \mu\mathbf{F}\mathbf{E} + \lambda(\text{tr}\mathbf{E})\mathbf{F}. \tag{5.22}$$

As-Rigid-As-Possible

As-Rigid-As-Possible (ARAP) energy, presented in Sec. 3.4.2 can be expanded to

$$\begin{aligned}\Psi_{\text{ARAP}} &= \frac{\mu}{2}\|\mathbf{F} - \mathbf{R}\|_F^2\\ &= \frac{\mu}{2}\left(\|\mathbf{F}\|_F^2 + \|\mathbf{R}\|_F^2 - 2\text{tr}\left(\mathbf{F}^T\mathbf{F}\right)\right)\\ &= \frac{\mu}{2}\left(\|\mathbf{F}\|_F^2 + \|\mathbf{R}\|_F^2 - 2\text{tr}\left(\mathbf{S}\right)\right),\end{aligned} \tag{5.23}$$

where $\mathbf{F} = \mathbf{R}\mathbf{S} \Rightarrow \mathbf{S} = \mathbf{F}^T\mathbf{R}$ (since $\mathbf{S}$ is symmetric). $\mathbf{P}_{\text{ARAP}}$ is then:

$$\mathbf{P}_{\text{ARAP}} = \mu(\mathbf{F} - \mathbf{R}). \tag{5.24}$$

A pretty easy $\mathbf{P}$ again!

Bonet-Wood Neo-Hookean

There are many energies that call themselves *'Neo-Hookean'*. One of the more popular ones is the one from the Bonet-Wood book [6]:

$$\Psi_{\text{BW08}} = \frac{\mu}{2}(\|\mathbf{F}\|_F^2 - 3) - \mu \ln(J) + \frac{\lambda}{2}(\ln(J))^2. \tag{5.25}$$

This is a bit more involved, so I'll jump to the result. Recall that the volume change of $\mathbf{F}$ is $J = \det \mathbf{F}$, so $\mathbf{P}$ of Ψ_{BW08} is

$$\mathbf{P}_{\text{BW08}} = \mu \left(\mathbf{F} - \frac{1}{J} \frac{\partial J}{\partial \mathbf{F}} \right) + \lambda \frac{\ln J}{J} \frac{\partial J}{\partial \mathbf{F}}. \tag{5.26}$$

A new term appears here: $\frac{\partial J}{\partial \mathbf{F}}$ is the gradient of J. In 3D, it can be written in terms of the *columns* of $\mathbf{F}$:

$$\mathbf{F} = \left[\begin{array}{c|c|c} & & \\ \mathbf{f}_0 & \mathbf{f}_1 & \mathbf{f}_2 \\ & & \end{array} \right]. \tag{5.27}$$

With the identity

$$J = \mathbf{f}_0 \cdot (\mathbf{f}_1 \times \mathbf{f}_2), \tag{5.28}$$

we can define the following convenient shorthand for $\frac{\partial J}{\partial \mathbf{F}}$:

$$\frac{\partial J}{\partial \mathbf{F}} = \left[\begin{array}{c|c|c} & & \\ \mathbf{f}_1 \times \mathbf{f}_2 & \mathbf{f}_2 \times \mathbf{f}_0 & \mathbf{f}_0 \times \mathbf{f}_1 \\ & & \end{array} \right]. \tag{5.29}$$

5.2.2 The next step

Computing forces is enough to get a simulator off the ground that does explicit time integration, but that just doesn't cut it in real-time. We want large timesteps, and as we discussed earlier, this requires some implicit timestepping scheme.

Such schemes, e.g. *backward Euler method* (Sec. 3.3.2) require the computation of the *force gradients*, i.e. $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$. All the tensor stuff we just did to get the $\mathbf{P}$s, just becomes so much more involved if you try to get the gradient of it. It'll take some work to make force gradient computation equally easy and pretty.

5.3 Computing Force Gradients

Let's recall that we've computed forces from the strain energy function as

$$\mathbf{f} = -v \frac{\partial \Psi}{\partial \mathbf{x}}. \tag{5.30}$$

It's pretty straightforward from this that we can calculate the *force gradients* as

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = -v \frac{\partial^2 \Psi}{\partial \mathbf{x}^2}. \tag{5.31}$$

In case of the force computation, the chain rule helped us to simplify the problem to

$$\frac{\partial \Psi}{\partial \mathbf{x}} = \frac{\partial \Psi}{\partial \mathbf{F}} : \frac{\partial \mathbf{F}}{\partial \mathbf{x}}. \tag{5.32}$$

This baked all the difficulty into the energy-agnostic tensor $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ that we only have to derive once. Then for each energy we only have to deal with the relatively easy $\frac{\partial \Psi}{\partial \mathbf{F}} \in \mathfrak{R}^{3\times 3}$ (a.k.a. $\mathbf{P}$).

Can we do something similar for the force gradient? Sure we can! Using the chain rule yet again, we arrive at

$$\frac{\partial^2 \Psi}{\partial \mathbf{x}^2} = \frac{\partial \mathbf{F}^T}{\partial \mathbf{x}} \frac{\partial^2 \Psi}{\partial \mathbf{F}^2} \frac{\partial \mathbf{F}}{\partial \mathbf{x}}. \tag{5.33}$$

That is, we take the *Hessian* of the strain energy function and left- and right-multiply it with the static 3rd-order tensor $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$.

5.3.1 The Mental Image of The Energy Hessian

The *Jacobian* of the strain energy function, $\frac{\partial \Psi}{\partial \mathbf{F}}$ is already the matrix $\mathbf{P}(\mathbf{F}) \in \mathfrak{R}^{3\times 3}$. Taking the derivate of Ψ yet again yields a 4th-order tensor. It could be written like $\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}$ as before, but $\frac{\partial \mathbf{P}}{\partial \mathbf{F}}$ means the same. We can write more explicitly

$$\frac{\partial^2 \Psi}{\partial \mathbf{F}^2} = \frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}} = \begin{bmatrix} \begin{bmatrix} \frac{\partial \mathbf{P}}{\partial f_{00}} \\ \frac{\partial \mathbf{P}}{\partial f_{10}} \\ \frac{\partial \mathbf{P}}{\partial f_{20}} \end{bmatrix} & \begin{bmatrix} \frac{\partial \mathbf{P}}{\partial f_{01}} \\ \frac{\partial \mathbf{P}}{\partial f_{11}} \\ \frac{\partial \mathbf{P}}{\partial f_{21}} \end{bmatrix} & \begin{bmatrix} \frac{\partial \mathbf{P}}{\partial f_{02}} \\ \frac{\partial \mathbf{P}}{\partial f_{12}} \\ \frac{\partial \mathbf{P}}{\partial f_{22}} \end{bmatrix} \end{bmatrix}. \tag{5.34}$$

Just like in the 3rd-order case, the bracketed $\frac{\partial \mathbf{P}}{\partial f_{ij}}$ are matrices, and they are entries in a heigher-order tensor. As the 3rd-order tensor was a *vector of matrices*, the 4th-order tensor is a *matrix of matrices*. See Fig. 5.2 for visualisation. The double-contraction operation looks quite similar to the 3rd-order case, except instead of producing a vector, the results are arranged into a matrix:

$$\begin{aligned} \mathbb{A} : \mathbf{B} &= \begin{bmatrix} \begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} & \begin{bmatrix} a_8 & a_{10} \\ a_9 & a_{11} \end{bmatrix} \\ \begin{bmatrix} a_4 & a_6 \\ a_5 & a_7 \end{bmatrix} & \begin{bmatrix} a_{12} & a_{14} \\ a_{13} & a_{15} \end{bmatrix} \end{bmatrix} : \begin{bmatrix} b_0 & b_2 \\ b_1 & b_3 \end{bmatrix} \\ &= \begin{bmatrix} (a_0 b_0 + a_1 b_1 + a_2 b_2 + a_3 b_3) & (a_8 b_0 + a_9 b_1 + a_{10} b_2 + a_{11} b_3) \\ (a_4 b_0 + a_5 b_1 + a_6 b_2 + a_7 b_3) & (a_{12} b_0 + a_{13} b_1 + a_{14} b_2 + a_{15} b_3) \end{bmatrix}. \end{aligned} \tag{5.35}$$

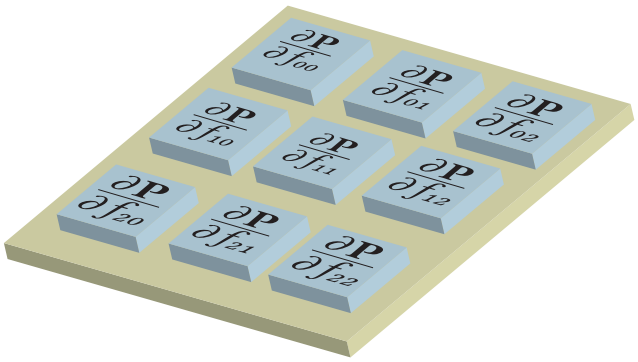


Figure 5.2: Thinking about 4^{th}-order tensors as a matrix of matrices.

Flattening the tensor

$$\mathbb{C} = \left[\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} 9 & 11 \\ 10 & 12 \end{bmatrix} \right] \left[\begin{bmatrix} 5 & 7 \\ 6 & 8 \end{bmatrix} \begin{bmatrix} 13 & 15 \\ 14 & 16 \end{bmatrix}\right] = \begin{bmatrix} [\mathbf{C}_{00}] & [\mathbf{C}_{01}] \\ [\mathbf{C}_{10}] & [\mathbf{C}_{11}] \end{bmatrix}, \tag{5.36}$$

requires first flattening in *column-wise order*, and then each matrix in turn:

$$\text{vec}(\mathbb{C}) = \left[\begin{array}{c|c|c|c} \text{vec}(\mathbf{C}_{00}) & \text{vec}(\mathbf{C}_{10}) & \text{vec}(\mathbf{C}_{01}) & \text{vec}(\mathbf{C}_{11}) \end{array}\right] = \begin{bmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & 10 & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{bmatrix}. \tag{5.37}$$

Taking the force gradient will require to multiply a 4^{th}-order tensor with a 3^{rd}-order one. Rather than defining the operation explicitly in 'tensor form', we are going to use the flattened matrix representation for that. Not only will this be easier to think about, but we will see some interesting structures appear.

5.3.2 Gradient Computation

Without further ado, here is the vectorized version of the force Jacobian which we are going to use through this text:

$$\frac{\partial^2 \Psi}{\partial \mathbf{x}^2} = \text{vec}\left(\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right)^T \text{vec}\left(\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}\right) \text{vec}\left(\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right). \tag{5.38}$$

As I have already mentioned many times, we got the formula for the $\text{vec}\left(\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right)$, so *'all we need'* is to derive $\text{vec}\left(\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}\right)$.

It certainly is all we need! However, if you try to derive it for all the energy functions out there, it's going to cost you a lot of tedious tensor manipulations. It's possible, but it's just too painful.

We are lucky, because there's a better way to deal with this. We can use an alternative representation of the energy function called *Cauchy-Green invariants*. It's going to provide us with a much simpler scheme to derive the force Jacobians.

5.4 The Cauchy-Green Invariants

In our simulator, we've restricted ourselves not only for conservative potential energies, but we are also going to use exclusively *isotropic materials*. Isotropy is defined by requiring the constitutive behavior to be identical in any material direction. A more *'mathematical'* definition could state that the energy function's behavior is *invariant under rotation.* This implies that the relationship between Ψ and $\mathbf{F}$ must be independent of the material axes chosen and, consequently, Ψ can be fully described by the Cauchy-Green invariants I_C, II_C, and III_C. These invariants arise from the characteristic polynomial of $\mathbf{C} = \mathbf{F}^T\mathbf{F}$, as follows:

$$\begin{aligned} I_\mathrm{C} &= \mathrm{tr}\mathbf{C}, \\ II_\mathrm{C} &= \mathrm{tr}\mathbf{C}^2, \\ III_\mathrm{C} &= \det\mathbf{C} = J^2. \end{aligned} \tag{5.39}$$

But, we are going to use them in the following form:

$$\begin{aligned} I_\mathrm{C} &= \|\mathbf{F}\|_F^2, \\ II_\mathrm{C} &= \|\mathbf{F}^T\mathbf{F}\|_F^2, \\ III_\mathrm{C} &= \det\left(\mathbf{F}^T\mathbf{F}\right). \end{aligned} \tag{5.40}$$

Why is this specific representation beneficial for us? First, to make the invariants usable, we need to *rewrite* each energy function using them. For e.g. the St. Venant Kirchhoff this means

$$\begin{aligned} \Psi_{\mathrm{StVK,stretch}} &= \|\mathbf{E}\|_F^2 \\ &= \frac{1}{4}\|\mathbf{F}^T\mathbf{F} - \mathbf{I}\|_F^2 \\ &= \frac{1}{4}\left(\|\mathbf{F}^T\|_F^2 - 2\mathrm{tr}\left(\mathbf{F}^T\mathbf{F}\right) + \|\mathbf{I}\|_F^2\right) \\ &= \frac{1}{4}II_\mathrm{C} - \frac{1}{2}I_\mathrm{C} + 3. \end{aligned} \tag{5.41}$$

We can do this for *almost* any energy! This is good news, because we only got 3 invariants! If we derive all the invariants' gradients $\mathbb{G}_x$, and Hessians $\mathbb{H}_x$, we can arrive at a *generic representation* of the force Jacobian by using the chain rule on $\frac{\partial^2\Psi}{\partial\mathbf{F}^2}$

$$\frac{\partial^2\Psi}{\partial\mathbf{F}^2} = \frac{\partial^2\Psi}{\partial I_C^2}\mathbb{G}_I + \frac{\partial\Psi}{\partial I_C}\mathbb{H}_I + \frac{\partial^2\Psi}{\partial II_C^2}\mathbb{G}_{II} + \frac{\partial\Psi}{\partial II_C}\mathbb{H}_{II} + \frac{\partial^2\Psi}{\partial III_C^2}\mathbb{G}_{III} + \frac{\partial\Psi}{\partial III_C}\mathbb{H}_{III}. \tag{5.42}$$

Here, for each invariant $x \in \{I_\mathrm{C}, II_\mathrm{C}, III_\mathrm{C}\}$, the gradient is $\mathbb{G}_x = \frac{\partial x}{\partial\mathbf{F}}$, while the Hessian is $\mathbb{H}_x = \frac{\partial^2 x}{\partial\mathbf{F}^2}$. We can define the energy Hessian in a bit more compact, but definitely more dull form as

$$\frac{\partial^2\Psi}{\partial\mathbf{F}^2} = \sum_{x\in\{I_\mathrm{C},II_\mathrm{C},III_\mathrm{C}\}} \frac{\partial^2\Psi}{\partial x^2}\mathbb{G}_x + \frac{\partial\Psi}{\partial x}\mathbb{H}_x. \tag{5.43}$$

This is a *complete rogue's gallery.* The $\mathbb{G}_x$ and $\mathbb{H}_x$ terms fully characterize the energy – there is no other term left! If we can work them out, all that's left for us is to derive the scalar derivative terms – all the $\frac{\partial\Psi}{\partial x}$s and $\frac{\partial^2\Psi}{\partial x^2}$s – in case we want to get the Hessian of a new energy.

5.4.1 Generic Invariant Gradients and Hessians

Deriving the $\mathbb{G}_x$ and $\mathbb{H}_x$ terms definitely requires some effort. But, if you do it once, you can use it for any energy. For the sake of completeness, I will list all the final results of the derivations here, altough I will omit the actual derivations themselves. The reader can refer to [15] for the complete calculations.

As we are going to use the *vectorized* version of the energy Hessian following Eq. 5.38, we have to first rewrite the generic Hessian as

$$\text{vec}\left(\frac{\partial^2\Psi}{\partial\mathbf{F}^2}\right) = \frac{\partial^2\Psi}{\partial I_{\text{C}}^2}\mathbf{g}_I\mathbf{g}_I^T + \frac{\partial\Psi}{\partial I_{\text{C}}}\mathbf{H}_I^T + \frac{\partial^2\Psi}{\partial II_{\text{C}}^2}\mathbf{g}_{II}\mathbf{g}_{II}^T + \frac{\partial\Psi}{\partial II_{\text{C}}}\mathbf{H}_{II}^T + \frac{\partial^2\Psi}{\partial III_{\text{C}}^2}\mathbf{g}_{III}\mathbf{g}_{III}^T + \frac{\partial\Psi}{\partial III_{\text{C}}}\mathbf{H}_{III}^T. \tag{5.44}$$

Here $\text{vec}\,(\mathbb{G}_x) = \mathbf{g}_x\mathbf{g}_x^T$ and $\text{vec}\,(\mathbb{H}_x) = \mathbf{H}_x$. Then, all the $\mathbf{g}_x$ and $\mathbf{H}_x$ terms can be defined as follows:
First Invariant

$$\mathbf{g}_I = \text{vec}\left(\frac{\partial I_{\text{C}}}{\partial\mathbf{F}}\right) = 2\text{vec}\,(\mathbf{F}) \tag{5.45}$$

$$\mathbf{H}_I = \text{vec}\left(\frac{\partial^2 I_{\text{C}}}{\partial\mathbf{F}^2}\right) = 2\mathbf{I}_{9\times9} \tag{5.46}$$

Second Invariant

$$\mathbf{g}_{II} = 4\text{vec}\,(\mathbf{FE})\,, \tag{5.47}$$

$$\mathbf{H}_{II} = 4\left(\mathbf{I}_{3\times3}\otimes\mathbf{F}\mathbf{F}^T + \mathbf{F}^T\mathbf{F}\otimes\mathbf{I}_{3\times3} + \mathbf{D}\right), \tag{5.48}$$

where $\otimes$ denotes the Kronecker product, while $\mathbf{D}$ is

$$\mathbf{D} = \begin{bmatrix} \mathbf{f}_0\mathbf{f}_0^T & \mathbf{f}_1\mathbf{f}_0^T & \mathbf{f}_2\mathbf{f}_0^T \\ \mathbf{f}_0\mathbf{f}_1^T & \mathbf{f}_1\mathbf{f}_1^T & \mathbf{f}_2\mathbf{f}_1^T \\ \mathbf{f}_0\mathbf{f}_2^T & \mathbf{f}_1\mathbf{f}_2^T & \mathbf{f}_2\mathbf{f}_2^T \end{bmatrix}. \tag{5.49}$$

The $\mathbf{f}_i$s here are the columns of $\mathbf{F}$, as of Eq. 5.27.
Third invariant We have already derived a fundamental building block for the third invariant. $\frac{\partial J}{\partial\mathbf{F}}$ appeared once in the Bonet-Wood Neo-Hookean Piola-Kirchhoff stress tensor (Eq. 5.26), and we are going to define

$$\mathbf{g}_J = \text{vec}\left(\frac{\partial J}{\partial\mathbf{F}}\right) = \text{vec}\left(\left[\begin{array}{c|c|c} \mathbf{f}_1\times\mathbf{f}_2 & \mathbf{f}_2\times\mathbf{f}_0 & \mathbf{f}_0\times\mathbf{f}_1 \end{array}\right]\right). \tag{5.50}$$

We are also going to need

$$\mathbf{H}_J = \begin{bmatrix} \mathbf{0} & -\hat{\mathbf{f}}_2 & -\hat{\mathbf{f}}_1 \\ \hat{\mathbf{f}}_2 & \mathbf{0} & -\hat{\mathbf{f}}_0 \\ -\hat{\mathbf{f}}_1 & \hat{\mathbf{f}}_0 & \mathbf{0} \end{bmatrix}, \tag{5.51}$$

using the hat operator $\hat{x}$, which turns a vector into a cross-product matrix:

$$\hat{\mathbf{x}} = \begin{bmatrix} 0 & -x_2 & x_1 \\ x_2 & 0 & -x_0 \\ -x_1 & x_0 & 0 \end{bmatrix}. \tag{5.52}$$

With these in hand, the gradient and Hessian of the third invariant is

$$\mathbf{g}_{III} = 2 \det J \cdot \mathbf{g}_J, \tag{5.53}$$

$$\mathbf{H}_{III} = 2\mathbf{g}_J\mathbf{g}_J^T + 2 \det J \cdot \mathbf{H}_J. \tag{5.54}$$

5.4.2 Force Jacobian the Cauchy-Green Way

There are now three steps to derive the Hessian of an energy:

1. Re-write your energy in terms of I_C, II_C, and III_C.
2. Derive the scalar derivatives. Scalar! Derivates! Just mash them into Wolfram Alpha!
3. Plug the results into Eq. 5.44. You're all done.

5.4.3 Examples

St. Venant-Kirchhoff Stretching

Let's try it out on the stretching term from St. Venant-Kirchhoff:

$$\Psi_{\mathrm{StVK,stretch}} = \|\mathbf{E}\|_F^2. \tag{5.55}$$

Step 1: Rewrite using invariants. We already did this in Eq. 5.41; the result is

$$\Psi_{\mathrm{StVK,stretch}} = \frac{1}{4}II_\mathrm{C} - \frac{1}{2}I_\mathrm{C} + 3. \tag{5.56}$$

Step 2: Take the invariant derivatives. Here they are:

$$\frac{\partial \Psi}{\partial I_\mathrm{C}} = -\frac{1}{2}, \qquad \frac{\partial^2 \Psi}{\partial I_\mathrm{C}^2} = 0, \tag{5.57}$$

$$\frac{\partial \Psi}{\partial II_\mathrm{C}} = \frac{1}{4}, \qquad \frac{\partial^2 \Psi}{\partial II_\mathrm{C}^2} = 0, \tag{5.58}$$

$$\frac{\partial \Psi}{\partial II_\mathrm{C}} = 0, \qquad \frac{\partial^2 \Psi}{\partial II_\mathrm{C}^2} = 0. \tag{5.59}$$

Okay this is easy! Almost all of them are zero.

Step 3: Plug the results into Eq. 5.44.

$$\begin{aligned} \mathrm{vec}\left(\frac{\partial^2 \Psi_{\mathrm{StVK,stretch}}}{\partial \mathbf{F}^2}\right) &= \frac{1}{4}\mathbf{H}_{II} - \frac{1}{2}\mathbf{H}_I \\ &= \frac{1}{4}\mathbf{H}_{II} - \mathbf{I}_{9\times 9} \end{aligned} \tag{5.60}$$

That went pretty well! What about ARAP?

5.4.4 As-Rigid-As-Possible: Things Go Terribly Wrong

From the title you might guess that something odd is going to happen with ARAP. Let's find it out! ARAP can be expanded as

$$\begin{aligned}\Psi_{\text{ARAP}} &= \frac{\mu}{2}\|\mathbf{F}-\mathbf{R}\|_F^2 \\ &= \|\mathbf{F}\|_F^2 - 2\text{tr}\left(\mathbf{F}^T\mathbf{R}\right) + \|\mathbf{R}\|_F^2 \\ &= I_{\text{C}} - 2\text{tr}\left(\mathbf{F}^T\mathbf{R}\right) + 3.\end{aligned} \tag{5.61}$$

Hang on a minute! What *is* $\text{tr}\left(\mathbf{F}^T\mathbf{R}\right)$? It does not correspond to any of the Cauchy-Green invariants!

To get to the bottom of this, the problem is going to boil down to the fact that what we are trying to take the symbolic derivative of something ($\mathbf{R}$) that is purely numerical. But let's not rush that far ahead just yet; first we'll elaborate a bit on this $\text{tr}\left(\mathbf{F}^T\mathbf{R}\right)$ term.

5.5 A New Set of Invariants?

This non-cooperative term, $\text{tr}\left(\mathbf{F}^T\mathbf{R}\right)$, looks almost like

$$I_{\text{C}} = \text{tr}\left(\mathbf{F}^T\mathbf{F}\right), \tag{5.62}$$

which is already pretty suspicious! Furthermore, we can use the polar decomposition, $\mathbf{F} = \mathbf{RS}$, to reorder this weird term to

$$\text{tr}\left(\mathbf{F}^T\mathbf{R}\right) = \text{tr}\left(\mathbf{S}^T\right) = \text{tr}\left(\mathbf{S}\right). \tag{5.63}$$

What if we just... added this to our gallery of invariants? Is it a sensible question to ask? In what follows, we are going to look at invariants from two different perspectives, in order to understand them intuitively: we will examine their *rotation removing property*, as well as their straightforward *geometric interpretation*.

5.5.1 Invariants as Rotation Removers

There are two very important properties of the energy functions: they should be *invariant* to any rigid body *translations* and *rotations*. If an element has been merely translated or rotated, its deformation score should show up as zero. We've seen in Eq. 4.8, if $\mathbf{F} = \mathbf{I}$, $\mathbf{F}$ corresponds to a pure translation. In case of the rotation invariance property, $\mathbf{F}$ needs to be a pure rotation matrix, e.g.

$$\mathbf{F}(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}. \tag{5.64}$$

We have to design our energy functions carefully in order to get $\Psi(\mathbf{F}) = 0$ in both cases. We have actually already seen two fundamentally different ways to deal with this.

The St. Venant-Kirchhoff Way

The stretching part of the St. Venant-Kirchhoff energy was

$$\Psi_{\text{StVK,stretch}} = \|\mathbf{E}\|_F^2 = \frac{1}{2}\|\mathbf{F}^T\mathbf{F} - \mathbf{I}\|_F^2. \tag{5.65}$$

If $\mathbf{F} = \mathbf{I}$, $\Psi_{\text{StVK,stretch}} = 0$ so it's definitely translationally invariant, but what about the rotational invariance? We can exploit a neat linear algebra identity here, that is, if $\mathbf{F}$ is a pure rotation, then $\mathbf{F}^T\mathbf{F} = \mathbf{I}$. Plugging this back to Eq. 5.65, we have $\mathbf{I} - \mathbf{I} = \mathbf{0}$. Cool! With the help of the polar decomposition $\mathbf{F} = \mathbf{RS}$ (Sec. 4.1.4) we can explicitly see the moment the rotation gets burned off:

$$\begin{aligned}\mathbf{F}^T\mathbf{F} &= (\mathbf{RS})^T\mathbf{RS} = \mathbf{S}^T\mathbf{R}^T\mathbf{RS} \\ &= \mathbf{S}^T\mathbf{IS} = \mathbf{S}^T\mathbf{S} \\ &= \mathbf{S}^2.\end{aligned} \tag{5.66}$$

We just found a new form of I_{C}, which is

$$I_{\text{C}} = \text{tr}\left(\mathbf{F}^T\mathbf{F}\right) = \text{tr}\left(\mathbf{S}^2\right), \tag{5.67}$$

and the StVK energy can be rewritten as

$$\Psi_{\text{StVK,stretch}} = \frac{1}{2}\|\mathbf{S}^2 - \mathbf{I}\|_F^2. \tag{5.68}$$

The As-Rigid-As-Possible Way

In Section 3.4.2, we introduced a fairly unortodox energy function: the As-Rigid-As-Possible or ARAP energy comes from geometry processing, and it has a distinctly different way of dealing with rotation removal.

The rotational part of $\mathbf{F}$, $\mathbf{R}$, is factorized from the polar decomposition, then it's simply substracted from $\mathbf{F}$ before its Frobenius norm is taken:

$$\Psi_{\text{ARAP}} = \frac{\mu}{2}\|\mathbf{F} - \mathbf{R}\|_F^2. \tag{5.69}$$

If $\mathbf{F} = \mathbf{I}$, or $\mathbf{F}$ is a pure rotation, we get the 0 valued energy. Score! This surely feels like a hack, but it works pretty well!

Similarly to the StVK energy, we can do some tensor algebra trickery to transfrom it into a more interesting form. We can use the fact that the Frobenius norm does not change under rotation to burn off $\mathbf{R}$ in this case as well:

$$\begin{aligned}\Psi_{\text{ARAP}} &= \|\mathbf{F} - \mathbf{R}\|_F^2 \\ &= \|\mathbf{R}^T(\mathbf{F} - \mathbf{R})\|_F^2 \\ &= \|\mathbf{R}^T(\mathbf{RS} - \mathbf{R})\|_F^2 \\ &= \|\mathbf{S} - \mathbf{I}\|_F^2.\end{aligned} \tag{5.70}$$

This almost looks like $\frac{1}{2}\|\mathbf{S}^2 - \mathbf{I}\|_F^2$! How much does that square matters though?

Comparing the Two Ways

If we want to *really* know what's going in a matrix, it's a pretty good idea to utilize SVD. (See Section 4.1.4.) The SVD of $\mathbf{F} = \mathbf{U}\Sigma\mathbf{V}^T$, and the entries of the diagonal matrix, Σ measure *exactly* how much stretching is going on along each of the 3D directions.

We can write both energies in terms of Σ, but yet again comes an obscene amount of algebra, which I'm going to omit here. You can look it up in [15] at page 53. In summary, we have

$$\Psi_{\text{StVK,stretch}} = \frac{1}{2}\|\Sigma^2 - \mathbf{I}\|_F^2, \tag{5.71}$$

$$\Psi_{\text{ARAP}} = \|\Sigma - \mathbf{I}\|_F^2. \tag{5.72}$$

Ignoring that $\frac{1}{2}$ in front of $\Psi_{\text{StVK,stretch}}$ – as we are looking for *qualitatively* different behaviours – the only real difference is that StVK squares all the singular values, while ARAP doesn't. Interesting! Summing this all up, we have a new alias for I_C by exploiting $\mathbf{S} = \mathbf{V}^T\Sigma\mathbf{V}$:

$$I_C = \text{tr}\left(\mathbf{F}^T\mathbf{F}\right) = \text{tr}\left(\mathbf{S}^2\right) = \text{tr}\left(\Sigma^2\right), \tag{5.73}$$

while that ill-behaving term of ARAP becomes

$$\text{tr}\left(\mathbf{R}^T\mathbf{F}\right) = \text{tr}\left(\mathbf{S}\right) = \text{tr}\left(\Sigma\right). \tag{5.74}$$

When looking at solely the singular values Σ, $\text{tr}\left(\mathbf{R}^T\mathbf{F}\right)$ definitely looks something similar to I_C. Again, how important is that squaring though? To answer that, we'll need to look at the invariants from a different perspective.

5.5.2 Invariants as Geometric Measures

Recall that Σ from the SVD of $\mathbf{F}$, $\mathbf{F} = \mathbf{U}\Sigma\mathbf{V}^T$, represent the singular values of $\mathbf{F}$, which measure how much stretching is going on *exactly*.
Going back to the $\text{tr}\left(\Sigma^2\right)$ form of I_C, it works out to

$$I_C = \sigma_x^2 + \sigma_y^2 + \sigma_z^2, \tag{5.75}$$

where $\sigma_{x,y,z}$ are the singular values. This has a pretty straightforward geometric representation! As we discussed in Sec. 4.1.2, the matrix $\mathbf{F}$ characterizes the rotation and *scaling* of an infinitesimal volumetric piece of a solid. On the other hand, the singular values are the amount of stretching and squashing *along each axis*; see Fig. 5.3!

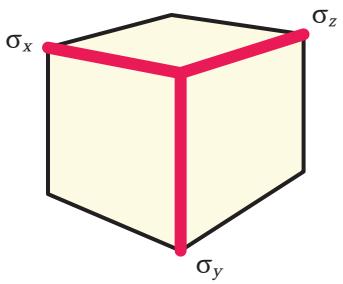


Figure 5.3: I_C measures the overall edge lengths of the entire cube. It i.e. sums up the squared lengths of each side of the cube.

So the invariant I_C is the *sum of the squared lengths of each side of the cube.* This is amazing! I actually haven't found any other material that described the Cauchy-Green invariants in such manner. We can now go ahead and define some similar term for both II_C and III_C. Both terms require some tweaking to get the final form presented in the followings. I omitted the derivations here, but you can look them up in the usual place, [15], page 55-56.
$II_C = \|\mathbf{F}^T\mathbf{F}\|_F^2$ works out to

$$II_C = \sigma_x^4 + \sigma_y^4 + \sigma_z^4, \tag{5.76}$$

which is the length of each side of the cube, raised to the fourth power. This doesn't differ much from I_C. To make it profitable, we need to fold it to an alternative form of

$$II_C^* = \frac{1}{2}(I_C - II_C). \tag{5.77}$$

II_C^* appears in e.g. [6], Example 6.5. Chugging through we will get

$$II_C^* = \left(\sigma_x\sigma_y\right)^2 + \left(\sigma_x\sigma_z\right)^2 + \left(\sigma_y\sigma_z\right)^2. \tag{5.78}$$

As you can see on Fig. 5.4, whereas I_C was the sum of the squared *lengths* of the cube *edges* II_C^* is the sum of the squared *areas* of the cube *faces.*

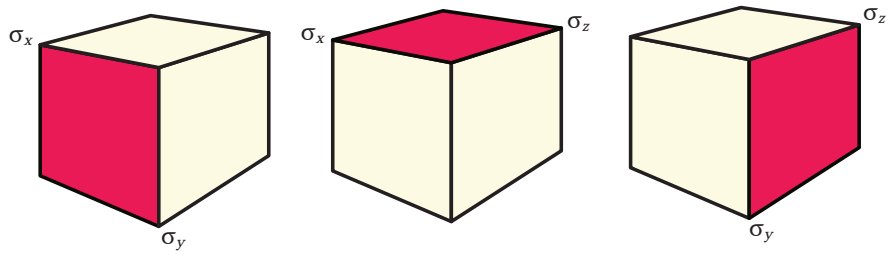


Figure 5.4: II_C measures the overall face areas of the cube. It i.e. sums up the squared areas of each side of the cube.

Finally, let's look at $III_C = \det\left(\mathbf{F}^T\mathbf{F}\right)$. By definition, the determinant of a matrix is the product of its singular values, so this one is relatively easy:

$$III_C = \left(\sigma_x\sigma_y\sigma_z\right)^2. \tag{5.79}$$

that is, III_C measures the square of the cube's volume (Fig. 5.5).

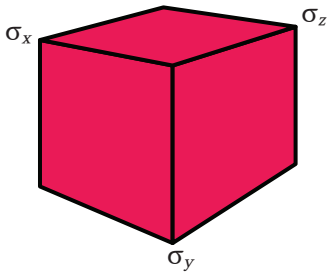


Figure 5.5: III_C measures squared volume of the cube.

Taken all together, all three invariants have a very intuitve geometric measure. It feels like a *fairly complete* way to describe how a small cube of material can deform, so it makes sense that the Cauchy-Green invariants is so popular among computational mechanists.

However, ARAP breaks this pattern; and it's a shame, as the use of rotation gradient $\mathbf{R}$ turned out to be pretty handy, when one designs new energies, e.g. McAdams et al. use it in their co-rotational formulation as well [18].

With all this knowledge in hand, let's look at our problem – describing $\mathrm{tr}\left(\mathbf{R}^T\mathbf{F}\right)$ – again.

5.6 S-based Invariants

I_C boiled down to

$$I_C = \mathrm{tr}\left(\Sigma^2\right), \tag{5.80}$$

while the non-cooperative term in ARAP can be expressed as

$$\mathrm{tr}\left(\mathbf{R}^T\mathbf{F}\right) = \mathrm{tr}\left(\mathbf{S}\right) = \mathrm{tr}\left(\Sigma\right). \tag{5.81}$$

The singular value version of I_C was

$$I_C = \sigma_x^2 + \sigma_y^2 + \sigma_z^2, \tag{5.82}$$

while the non-cooperative term takes the form.

$$\mathrm{tr}\left(\mathbf{S}\right) = \sigma_x + \sigma_y + \sigma_z. \tag{5.83}$$

This is the *unsquared version* of I_C! Finally, it becomes clear that **you can't use a sum of squared values to express a sum of unsquared values.** This is why ARAP can't be written in terms of the Cauchy-Green invariants. This strongly suggests that $\mathrm{tr}\left(\mathbf{S}\right)$ should be its own invariant:

$$\boxed{I_1 = \mathrm{tr}\left(\mathbf{S}\right).} \tag{5.84}$$

We essentially substituted $\mathbf{F}^T\mathbf{F}$ with $\mathbf{S}$. Can we do this to the other invariants as well? Doing so would reveal the new $\mathbf{S}$-based second and third invariant.

$$II_C = \mathrm{tr}\left(\mathbf{F}^T\mathbf{F}\mathbf{F}^T\mathbf{F}\right) \quad \rightarrow \quad I_2 = \mathrm{tr}\left(\mathbf{S}^2\right), \tag{5.85}$$

$$III_C = \det\left(\mathbf{F}^T\mathbf{F}\right) \quad \rightarrow \quad I_3 = \det\left(\mathbf{S}\right). \tag{5.86}$$

Is it a good set of invariants? Kim ([15], page 58) used these new invariants to express the original Cauchy-Green invariants. Doing so proved that the new invariants can describe a *super-set* of the phenomena that the Cauchy-Green ones could.

5.6.1 Does ARAP Work Now?

After all this work, let's try to write the ARAP energy in terms of our *new* invariants:

$$I_1 = \operatorname{tr} \mathbf{S}, \qquad I_2 = \operatorname{tr}\left(\mathbf{S}^2\right), \qquad I_3 = \det \mathbf{S}. \tag{5.87}$$

Can we do it? For the following computations, I will drop the $\frac{\mu}{2}$ term to make the derivations cleaner.

$$\begin{aligned} \Psi_{\text{ARAP}} &= \|\mathbf{F} - \mathbf{R}\|_F^2 \\ &= \|\mathbf{F}\|_F^2 - 2\operatorname{tr}\left(\mathbf{F}^T\mathbf{R}\right) + \|\mathbf{R}\|_F^2 \\ &= I_2 - 2I_1 + 3 \end{aligned} \tag{5.88}$$

So far so good! Let's chug ahead and calculate the PK1:

$$\begin{aligned} \frac{\partial \Psi_{\text{ARAP}}}{\partial \mathbf{F}} &= \frac{\partial}{\partial \mathbf{F}}\left(I_2 - 2I_1 + 3\right) \\ &= \frac{\partial I_2}{\partial \mathbf{F}} - 2\frac{\partial I_1}{\partial \mathbf{F}}. \end{aligned} \tag{5.89}$$

Since $I_2 = I_{\text{C}}$

$$\frac{\partial I_2}{\partial \mathbf{F}} = \frac{\partial I_{\text{C}}}{\partial \mathbf{F}} = 2\mathbf{F}, \tag{5.90}$$

while

$$\frac{\partial I_1}{\partial \mathbf{F}} = \frac{\partial \operatorname{tr}(\mathbf{S})}{\partial \mathbf{F}} = \frac{\partial \operatorname{tr}\left(\mathbf{R}\mathbf{F}^T\right)}{\partial \mathbf{F}} = \mathbf{R}, \tag{5.91}$$

so

$$\mathbf{P}_{\text{ARAP}} = 2(\mathbf{F} - \mathbf{R}). \tag{5.92}$$

This exactly matches Eq. 5.24 – if you multiply it with $\frac{\mu}{2}$. Cool! What about the Hessian? It will expand to

$$\begin{aligned} \frac{\partial^2 \Psi_{\text{ARAP}}}{\partial \mathbf{F}^2} &= 2\frac{\partial}{\partial \mathbf{F}}\left(\mathbf{F} - \mathbf{R}\right) \\ &= 2\left(\frac{\partial \mathbf{F}}{\partial \mathbf{F}} - \frac{\partial \mathbf{R}}{\partial \mathbf{F}}\right). \end{aligned} \tag{5.93}$$

Oh noo! An unfamiliar term again! What is this $\frac{\partial \mathbf{R}}{\partial \mathbf{F}}$? It's called the *rotation gradient*, but we didn't see anything like this before. And our brand new I_1 invariant doesn't help us at all. What now?

5.7 The Eigenmatrices of the Rotation Gradient

We have this fancy, new, more expressive set of invariants, but we're stuck again with the rotation gradient. The situation is even worse, as $\frac{\partial \mathbf{R}}{\partial \mathbf{F}} = \frac{\partial^2 I_1}{\partial \mathbf{F}^2}$, so if we can't figure out a good way to deal with this problem, then everything was for naught.

As I hinted already in Sec. 5.4.4, the core issue is, that *there isn't any method to obtain a tidy symbolic derivative of some numerical quantity* like $\mathbf{R}$. However, $\mathbf{R}$ *does indeed* will have a simple, clean structure; we just need to look at it from the right perspective.

The trick is going to be that the *eigendecomposition* of $\frac{\partial \mathbf{R}}{\partial \mathbf{F}}$ will be a simple structure. Smith et al. in [25] were able to come up with the *analytic, closed-form* representation of the eigenvectors and eigenvalues – which are usually packed into $\mathbf{Q}$ and $\mathbf{\Lambda}$. The rotation gradient then can be simply calculated as $\frac{\partial \mathbf{R}}{\partial \mathbf{F}} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$.

I think it's not the place where I need to stress how big of an achievement that is. And the researcher who found it, Theodore Kim, allegedly was just *'messing around in Matlab'* trying to *'plug in some easy-looking integers'* into the equations, until he *'found something that looked like a pattern'*. This process might sounds frighteningly informal to you, but as a – *hopefully soon to-be* – engineer, I found it fascinating – as it just works and it's also pretty efficient in code, and to me that's all that matters.

But first, to be sure we are all on the same page about *eigenvalues*, *eigenvectors*, *eigendecomposition*, and the slightly more exotic *eigenmatrices*, let's recap these linear algebra terms real quick.

5.7.1 Eigenvalues, Eigenvectors, Eigendecomposition

Everybody knows the basic eigenvalue problem:

$$\mathbf{A}\mathbf{q}_0 = \lambda_0 \mathbf{q}_0. \tag{5.94}$$

The eigenvalue λ_0 and the eigenvector $\mathbf{q}_0$ form an eigenpair of $\mathbf{A}$. The vector $\mathbf{q}_0$ is special because even after you push it through a multiply with $\mathbf{A}$, it remains exactly the same. Except, it was scaled by λ_0.

A geometrical definition could state, that an eigenvector points in a direction in which it is stretched by the matrix – or more like the *transformation* – and the eigenvalue is the factor by which it is stretched.

This means that the eigenvectors $\mathbf{q}_i$ and the corresponding eigenvalues λ_i of a matrix – *a.k.a. transform* – $\mathbf{A}$ completely characterize the matrix itself. Thus, you can recover matrix $\mathbf{A}$ from

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T. \tag{5.95}$$

where $\mathbf{Q}$'s i^{th} column correspons to an i^{th} eigenvector, $\mathbf{q}_i$. $\mathbf{\Lambda}$ is a diagonal matrix, whose diagonal elements are the corresponding eigenvalues, such that $\Lambda_{ii} = \lambda_i$.

5.7.2 What's an Eigenmatrix?

While everybody heard about the eigenvalues and eigenvectors, you might not have come across an eigenmatrix. For some 4^{th}-order tensor

$$\mathbb{A} = \begin{bmatrix} \begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} & \begin{bmatrix} a_8 & a_{10} \\ a_9 & a_{11} \end{bmatrix} \\ \begin{bmatrix} a_4 & a_6 \\ a_5 & a_7 \end{bmatrix} & \begin{bmatrix} a_{12} & a_{14} \\ a_{13} & a_{15} \end{bmatrix} \end{bmatrix}, \tag{5.96}$$

we define a similar eigenpair, $\{\lambda_0, \mathbf{Q}_0\}$, like in the matrix-world, but here we talk about an eigenmatrix, instead of an eigenvector. The equivalent eigenproblem then is defined as

$$\mathbb{A} : \mathbf{Q}_0 = \lambda_0 \mathbf{Q}_0, \tag{5.97}$$

where we used our favourite double-contraction operation instead of a plain matrix-vector multiply. This can be expanded to

$$\begin{aligned}\mathbb{A} : \mathbf{Q}_0 &= \begin{bmatrix} \begin{bmatrix} a_0 & a_2 \\ a_1 & a_3 \end{bmatrix} & \begin{bmatrix} a_8 & a_{10} \\ a_9 & a_{11} \end{bmatrix} \\ \begin{bmatrix} a_4 & a_6 \\ a_5 & a_7 \end{bmatrix} & \begin{bmatrix} a_{12} & a_{14} \\ a_{13} & a_{15} \end{bmatrix} \end{bmatrix} : \begin{bmatrix} q_0 & q_2 \\ q_1 & q_3 \end{bmatrix} \\ &= \begin{bmatrix} (a_0q_0 + a_1q_1 + a_2q_2 + a_3q_3) & (a_8q_0 + a_9q_1 + a_{10}q_2 + a_{11}q_3) \\ (a_4q_0 + a_5q_1 + a_6q_2 + a_7q_3) & (a_{12}q_0 + a_{13}q_1 + a_{14}q_2 + a_{15}q_3) \end{bmatrix} \\ &= \lambda_0 \begin{bmatrix} q_0 & q_2 \\ q_1 & q_3 \end{bmatrix} = \lambda_0 \mathbf{Q}_0.\end{aligned} \tag{5.98}$$

Again, this is essentially the same thing, as with the matrix eigenvalue-eigenvector problem: contracting $\mathbb{A}$ with $\mathbf{Q}_0$, $\mathbb{A}$ stays the same. Except it was scaled by λ_0.

Remember that vectorization process from Sec. 5.3.1, which turned this mighty 4^{th}-order tensor into a matrix? It was $\text{vec}(\mathbb{A}) = \mathbf{A}$. Now the thing is that the flattened eigenmatrix $\mathbf{Q}_0$ of a tensor $\mathbb{A}$ – which is a vector, of course – is going to be the eigenvector of the flattened tensor – which is a matrix. Are you still with me? It's much more understandable written like this:

$$\text{vec}(\mathbb{A})^T \, \text{vec}(\mathbf{Q}_0) = \mathbf{A}^T \mathbf{q}_0. \tag{5.99}$$

This is my favourite property of the vectorization process – it reveals that $\mathbf{A}\mathbf{q}_0 = \lambda_0 \mathbf{q}_0$ and $\mathbb{A} : \mathbf{Q}_0 = \lambda_0 \mathbf{Q}_0$ are essentially the same. Spelling out the whole thing verbosely yields:

$$\begin{aligned}\text{vec}(\mathbb{A})^T \, \text{vec}(\mathbf{Q}_0) = \mathbf{A}^T \mathbf{q}_0 &= \begin{bmatrix} a_0 & a_4 & a_8 & a_{12} \\ a_1 & a_5 & a_9 & a_{13} \\ a_2 & a_6 & a_{10} & a_{14} \\ a_3 & a_7 & a_{11} & a_{15} \end{bmatrix}^T \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} \\ &= \begin{bmatrix} a_0q_0 + a_1q_1 + a_2q_2 + a_3q_3 \\ a_4q_0 + a_5q_1 + a_6q_2 + a_7q_3 \\ a_8q_0 + a_9q_1 + a_{10}q_2 + a_{11}q_3 \\ a_{12}q_0 + a_{13}q_1 + a_{14}q_2 + a_{15}q_3 \end{bmatrix} \\ &= \lambda_0 \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} = \lambda_0 \mathbf{q}_0 = \lambda_0 \text{vec}(\mathbf{Q}_0).\end{aligned} \tag{5.100}$$

This property is very handy, because we don't need to come up with any new way to find the eigenmatrix of some tensor $\mathbb{A}$. You can use your favourite eigenvalue routine – be it Matlab, numpy, Eigen, or even LAPACK – and fold the $\{\lambda_i, \mathbf{q}_i\}$ pairs back into and eigenmatrix pair $\{\lambda_i, \mathbf{Q}_i\}$. But why do we even care about eigenmatrices, if they contain the exact same entries as the eigenvectors; just repackaged into a matrix form?

5.7.3 Structures Lurk in the Decomposition of an Eigenmatrix

The reason is that eigen*matrices* are – matrices! This means that we can apply a variety of matrix based tools that are just not available for vectors. Let's recall again that we have this SVD thing (Sec. 4.1.4) which proved to be in so useful already so many times. It was for $\mathbf{F}$:

$$\mathbf{F} = \mathbf{U}\Sigma\mathbf{V}^T. \tag{5.101}$$

We could rotate any matrix – e.g. $\mathbf{Q}_0$ – to the same space as $\mathbf{F}$ using $\mathbf{U}\mathbf{Q}_0\mathbf{V}^T$. This doesn't give any interpretable result, just a sea of meaningless numbers... But how about – following again Smith et al. [25] – rotating $\mathbf{Q}_0$ *out* of the space of $\mathbf{F}$ using

$$\mathbf{U}^T\mathbf{Q}_0\mathbf{V}. \tag{5.102}$$

This was *the trick*, which revealed that eigenmatrices of $\frac{\partial \mathbf{R}}{\partial \mathbf{F}}$ indeed have a simple clean structure. The whole thought process is documented in Section 5.4 in [15], so I will just jump to the final result now.

5.7.4 Building the Rotation Gradient

As the 3D rotation gradient is rank-3, we have the following three eigenpairs:

$$\lambda_0 = \frac{2}{\sigma_x + \sigma_y} \qquad \mathbf{Q}_0 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{5.103}$$

$$\lambda_1 = \frac{2}{\sigma_y + \sigma_z} \qquad \mathbf{Q}_1 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}\mathbf{V}^T \tag{5.104}$$

$$\lambda_2 = \frac{2}{\sigma_x + \sigma_z} \qquad \mathbf{Q}_2 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{5.105}$$

where again, σ_is, $\mathbf{U}$, and $\mathbf{V}$ comes from the SVD of $\mathbf{F}$. The matrices sandwiched between $\mathbf{U}$ and $\mathbf{V}$ are the twist matrices, corresponding to some infinitesimal rotation.

The $\frac{1}{\sqrt{2}}$ makes sense too. Eigenvectors have unit magnitude, and since $\mathbf{U}$ and $\mathbf{V}$ are already unitary matrices, the only things left to normalize are the 1 and -1 in the twist matrix. Since $\sqrt{1^2 + (-1)^2} = \sqrt{2}$, the normalization factor is $\frac{1}{\sqrt{2}}$. Neat, huh?

With the explicit λ_i and $\mathbf{Q}_i$ formulas, we arrive at a very simple form of the vectorized rotation gradient:

$$\mathrm{vec}\left(\frac{\partial \mathbf{R}}{\partial \mathbf{F}}\right) = \sum_{i=0}^{2} \lambda_i \mathrm{vec}(\mathbf{Q}_i)\mathrm{vec}(\mathbf{Q}_i)^T. \tag{5.106}$$

5.8 New Generic Hessian

As $\frac{\partial \mathbf{R}}{\partial \mathbf{F}} = \frac{\partial^2 I_1}{\partial \mathbf{F}^2}$, we now have everything in our hands to make a generic Hessian representation, just like in Sec. 5.4.1; but with the Smith et al. [25] invariants!
The Smith et al. invariants were

$$I_1 = \operatorname{tr}(\mathbf{S}), \qquad I_2 = \operatorname{tr}\left(\mathbf{F}^T\mathbf{F}\right), \qquad I_3 = \det \mathbf{F}. \tag{5.107}$$

and we now have the gradients ($\mathbf{g}_i$) and Hessians ($\mathbf{H}_i$) of each:

$$\begin{aligned}
\mathbf{g}_1 &= \operatorname{vec}(\mathbf{R}) & \mathbf{H}_1 &= \textstyle\sum_{i=0}^{2} \lambda_i \operatorname{vec}(\mathbf{Q}_i)\operatorname{vec}(\mathbf{Q}_i)^T \\
\mathbf{g}_2 &= \operatorname{vec}(2\mathbf{F}) & \mathbf{H}_2 &= 2\mathbf{I}_{9\times 9} \\
\mathbf{g}_J &= \operatorname{vec}\left(\left[\begin{array}{c|c|c} \mathbf{f}_1 \times \mathbf{f}_2 & \mathbf{f}_2 \times \mathbf{f}_0 & \mathbf{f}_0 \times \mathbf{f}_1 \end{array}\right]\right) & \mathbf{H}_J &= \begin{bmatrix} \mathbf{0} & -\hat{\mathbf{f}}_2 & -\hat{\mathbf{f}}_1 \\ \hat{\mathbf{f}}_2 & \mathbf{0} & -\hat{\mathbf{f}}_0 \\ -\hat{\mathbf{f}}_1 & \hat{\mathbf{f}}_0 & \mathbf{0} \end{bmatrix}
\end{aligned} \tag{5.108}$$

and the new generic Hessian is

$$\begin{aligned}
\operatorname{vec}\left(\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}\right) &= \frac{\partial^2 \Psi}{\partial I_1^2}\mathbf{g}_1\mathbf{g}_1^T + \frac{\partial \Psi}{\partial I_1}\mathbf{H}_1^T + \frac{\partial^2 \Psi}{\partial I_2^2}\mathbf{g}_2\mathbf{g}_2^T + \frac{\partial \Psi}{\partial I_2}\mathbf{H}_2^T + \frac{\partial^2 \Psi}{\partial I_3^2}\mathbf{g}_3\mathbf{g}_3^T + \frac{\partial \Psi}{\partial I_3}\mathbf{H}_3^T \\
&= \sum_{i=1}^{3} \frac{\partial^2 \Psi}{\partial I_i^2}\mathbf{g}_i\mathbf{g}_i^T + \frac{\partial \Psi}{\partial I_i}\mathbf{H}_i.
\end{aligned} \tag{5.109}$$

Finally, we can follow the very same three-step process as before:

1. Rewrite energies Ψ using I_1, I_2, and I_3.
2. Derive the scalar derivatives $\frac{\partial \Psi}{\partial I_1}$, $\frac{\partial^2 \Psi}{\partial I_1^2}$, $\frac{\partial \Psi}{\partial I_2}$, $\frac{\partial^2 \Psi}{\partial I_2^2}$, $\frac{\partial \Psi}{\partial I_3}$ and $\frac{\partial^2 \Psi}{\partial I_3^2}$.
3. Plug the result into Eq. 5.109.

5.8.1 Does ARAP Work Now?

Spoiler: it does! Again the ARAP energy was

$$\Psi_{\text{ARAP}} = \|\mathbf{F} - \mathbf{R}\|_F^2. \tag{5.110}$$

Step 1: Rewrite using invariants. We did all this mess just to do this:

$$\Psi_{\text{ARAP}} = I_2 - 2I_1 + 3. \tag{5.111}$$

Step 2: Take the invariant derivatives. Here they are:

$$\frac{\partial \Psi}{\partial I_1} = -2, \qquad \frac{\partial^2 \Psi}{\partial I_1} = 0, \tag{5.112}$$

$$\frac{\partial \Psi}{\partial I_2} = 1, \qquad \frac{\partial^2 \Psi}{\partial I_2} = 0, \tag{5.113}$$

$$\frac{\partial \Psi}{\partial I_3} = 0, \qquad \frac{\partial^2 \Psi}{\partial I_3} = 0. \tag{5.114}$$

Step 3: Plug the results into Eq. 5.109.

$$\text{vec}\left(\frac{\partial^2 \Psi_{\text{ARAP}}}{\partial \mathbf{F}^2}\right) = 2\mathbf{I}_{9\times 9} - 2\mathbf{H}_1 \tag{5.115}$$

Woah! Such a nice equation! And it's not just pretty, it's also very easy to implement, and if you have a nice SVD routine, it's also fast.

Thank YOU for following me on this journey into the inner workings of the Smith et al. invariants. In the next chapter we are going to build directly on the analytic eigenvalues of the rotation gradient, to find out another nice property of ARAP.

Chapter 6

Keeping the Hessian Positive Definite

After all this heavy-weight tensor algebra, you probably thought we are done. We finally have the energy Hessian a.k.a. the force Jacobian a.k.a. the tangent stiffness matrix; so all we need to do now, is to plug this into some timestepping scheme to arrive at some linear system $\mathbf{Ax} = \mathbf{b}$. And we are done! Just solve for $\mathbf{x}$!

Okay, you are right, we indeed just need to solve this $\mathbf{Ax} = \mathbf{b}$ for $\mathbf{x}$. But, since we are in a performance critical enviroment – remember the title of this thesis is *interactive* FE simulations – how we solve this system of equations *does* matter.

The go-to solution in Finite Element Analysis is to use some direct method, e.g. *LU factorization* of matrix $\mathbf{A}$ and solve the equations by backsubstitution. Such methods are great – they provide the exact solution of *any matrix* in a finite number of steps. However, in case of big matrices – and usually Finite Element matrices which consist of a couple thousand DoFs count as big ones – they get pretty slow.

We are in lucky, again – there is another way! Iterative methods, instead of directly solving $\mathbf{Ax} = \mathbf{b}$, starts at some initial value $\mathbf{x}_0$, and uses that to generate a sequence of improving approximate solutions. A typical example of iterative methods is the *conjugate gradient method*, what we are also going to use to solve the Finitie Element equilibrium. The process is explaned in the next section, (and visualized on Fig. 6.1, Fig. 6.2 and Fig. 6.3). We are going to exploit the fact that the resultant matrices are sparse – usually there are many more zeros in them than non-zeros – and *positive-definite*!

This is good, because the resulting matrix we've got is sparse and positive-definite, right? Well, yes, but no! If you've taken Finite Element classes, you'll know that $\mathbf{K}$ *is* positive-definite. However, the use of large timesteps produces substantial divergence from the steady state, leading to a symmetric linear system that is often indefinite. Which is very bad news and the latter part of this chapter is going to deal with this problem.

If it's the first time you're hearing about iterative methods for solving a linear system, I'm highly recommending you: 1. Shewchuk's infamous guide – *An Introduction to the Conjugate Gradient Method Without the Agonizing Pain* [23] – and 2. Appendix B, where I solve a simple 2×2 problem with the method of steepest descent.

6.1 Solving a Linear System Iteratively

6.1.1 Meaning of Matrix's Definiteness

Back to this definiteness – indefiniteness ordeal, what does it even mean if a matrix is definite or indefinite? I *always* prefer some type of visualization over a formula, so let's look at Fig. 6.1, where a plot of a positive definite, negative definite; singular and an indefinite matrix's quadratic form is shown. If you don't know what a quadratic form of some matrix is, please refer to Appendix B.

6.1.2 The Method of Steepest Descent

After looking at Fig. 6.1, you probably get the idea why we want positive definiteness: computing physics is a *minimization* problem most of the time. E.g. we want to find the global minima of the total potential energy function. If you've got something like Fig. 6.1a, you can imagine that you roll down a ball on that nice valley – down *is* the negative gradient of the surface – being careful that you *always* roll it down, up to the point that there is no more down. You can pull something like this off with a negative definite matrix, but definitely not with an indefinite one. What I just described is the method of steepest descent, which I also present of Fig. 6.2. And in Appendix B.

6.1.3 The Method of Conjugate Gradients

The example would run until it converges in Fig. 6.2. Not bad, however, note the zigzag path on Fig. 6.3. It appears because each gradient is *orthogonal* to the previous gradient. Wouldn't it be better if, every time we took a step, we got it right the first time?

In order to keep things short, most simulators use the method of Conjugate Gradient to solve the positive-definite, linear system. In a nutshell, while the method of steepest descent takes a step in the opposite direction of the gradient (Fig. 6.2, black), conjugate gradient steps in the direction of the conjugate vector (Fig. 6.2, red). I'm not going to derive the conjugate gradient method here, but instead would like to refer wholeheartedly to Shewchuk's explanation. [23]

6.2 Solving the Issue of Definiteness

What do we do with this definiteness-indefiniteness problem we've talked about? To give you a hint, there is this definition for a positive definite matrix:

$$\mathbf{x}^T\mathbf{A}\mathbf{x} \geq 0 \quad \forall \mathbf{x} \tag{6.1}$$

or if you are a regular human you can just say that *all of its eigenvalues are greater than, or equals to zero.* This is actually semi-positive definiteness. Another way to look at this is through the product $\mathbf{A}\mathbf{x} = \mathbf{b}$. Positive definiteness implies that the sign of each entry in $\mathbf{b}$ must always match the corresponding entry in $\mathbf{x}$. The matrix $\mathbf{A}$ is not allowed to flip the sign of any entry in $\mathbf{x}$, no matter what the entries in $\mathbf{x}$ are.

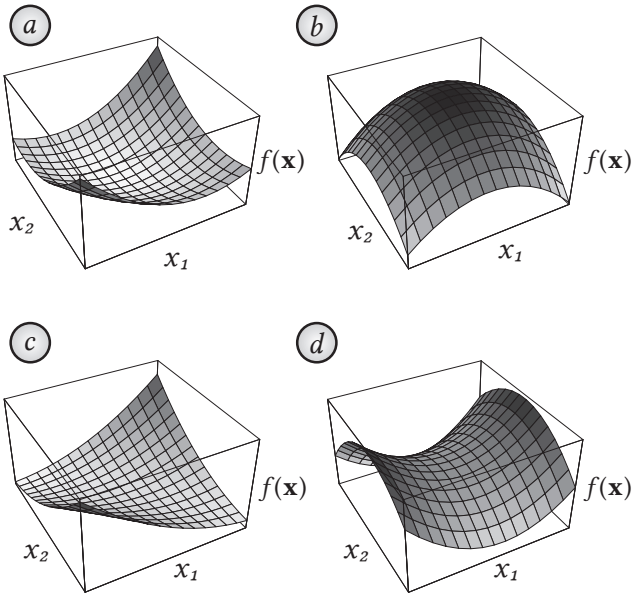


Figure 6.1: a – quadratic form for a positive definite matrix. b – for a negative definite matrix. c – for a singular (and positive-indefinite) matrix. A line that runs through the bottom of the valley is the set of solutions. d – for an indefinite matrix. Because the solution is a saddle point, steepest descent will not work. In three dimensions or higher, a singular matrix can also have a saddle.

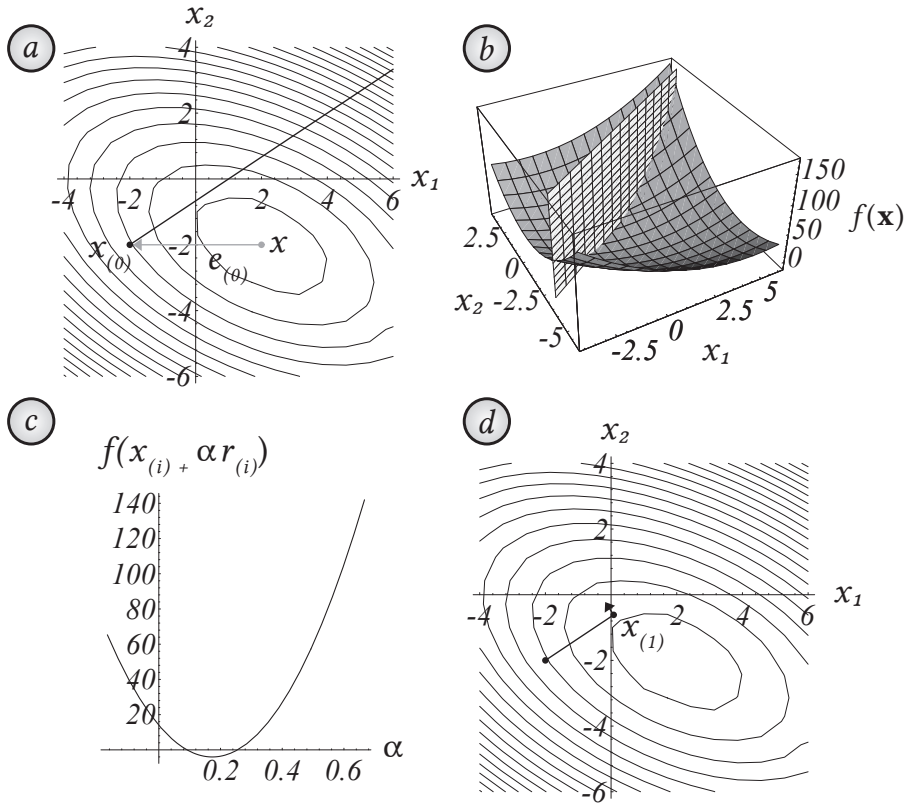


Figure 6.2: The method of Steepest Descent. a – Starting at $[-2, -2]^T$, take a step in the direction of steepest descent of f. b – Find the point on the intersection of these two surfaces that minimizes f. c – This parabola is the intersection of surfaces. The bottommost point is our target. d – The gradient at the bottommost point is orthogonal to the gradient of the previous step.

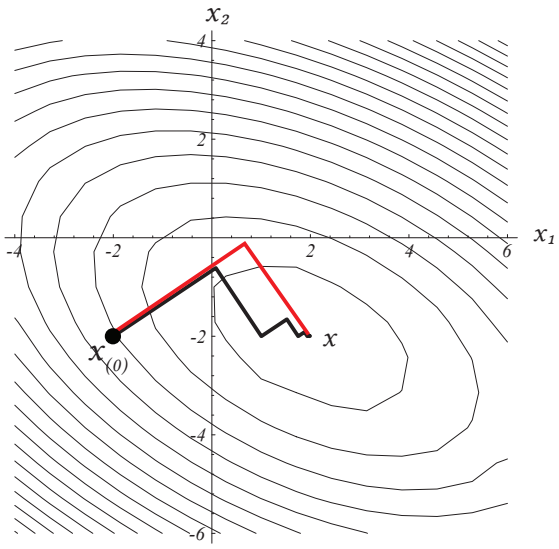


Figure 6.3: Black: The method of Steepest Descent starts at $[-2,-2]^T$ and converges at $[2,-2]^T$. Red: Method of Conjugate Gradient.

Here comes *the trick*: what if we *detect that the eigenvalue is less than zero*, we just *set it to be zero*? Surely we need all the eigenvalues and eigenvectors in order to reassemble the modified matrix, but wouldn't this eigenvalue sign be the source of all this trouble? The answer is: yes, and this will be the solution.

But how do we do that? One way would be to compute the eigendecomposition of the global Hessian. However, the eigendecomposition of an $\mathfrak{R}^{n\times n}$ matrix takes $O(n^3)$ steps while the conjugate gradient runs at $O(n^{\frac{3}{2}})$, so the cure is worse than the disease.

We can instead try per-element projection! If an element is indefinite, i.e. *any of its eigenvalues is less than 0*, then *clamp it to 0*. This would require the eigendecomposition of a bunch of 9×9, not the whole $n\times n$ system. The sum of semi-positive-definite matrices is known to also be semi-positive definite, so this strategy is sound.

6.3 Methods for Hessian Projection

This method of *eigenvalue clamping* is called Hessian projection in literature, and it had some notable contribution in the last couple of years. The thing is that since we are talking about the Hessian of specific, closed form energies, we can painstakingly analyze them, in order to make the problem simpler.

The method was first introduced by Teran et al. in [12] and [33]. They've successfully reduced the problem to probing a 3×3 and three 2×2 eigenproblem.[1] Their method was very innovative and important, but the use of the Cauchy-Green invariants made it limiting, due to the fact that it is insufficient to express stretch-based energies such as ARAP or the Co-rotational model.

This limitation was addressed in Stomakhin et al. in [29] by replacing the Cauchy-Green invariants with the singular values of the deformation gradient, however the inefficient numerical

[1]Teran later moved away from the field and started working with the Material Point Method; he was on the team developing the snow simulation for the Disney movie Frozen. [30] Such an amazing movie!

eigensolves for Hessian blocks remain. Xu et al. [35] improved these computations further by restricting the analysis to energies that satisfy the Valanis-Landel hypothesis. Unfortunately, many energies from geometry processing, such as MIPS [10] or Symmetric ARAP [27] do not fall into this category.

The work of McAdams et al. [18] presented an analytic solution for the indefiniteness of the Co-rotational energy. To do so, they've decomposed the 4^{th} order tensor defined by the energy Hessian into symmetric and skew-symmetric parts. This yields the eigenstructure of the Co-rotational model, albeit embedded inside 4^{th} order tensors.

Smith et al. [25] proposed a more general derivation that produces their eigenvalue expressions as a special case, additionally revealing the structure of the underlying eigenvectors. They've successfully aquired closed-form, analytic expression for 6 eigenpairs of the rank-9 Hessian. The first three eigenpairs can be computed from the eigendecomposition of a 3×3 matrix in the most general case, but for many popular distrotion energies, we can aquire closed-form expression as well.

6.4 Analytical Eigensystem of ARAP

Okay there are many nice articles about this Hessian projection thing, but what do they *actually* do? Well, we've already talked a lot about these eigenthingies in Sec. 5.7, when we tried to take the symbolic derivative of the rotation gradient:

$$\frac{\partial \mathbf{R}}{\partial \mathbf{F}} = \sum_{i=0}^{2} \lambda_i \text{vec}\left(\mathbf{Q}\right)_i \text{vec}\left(\mathbf{Q}\right)_i^T = \mathbf{H}_1, \tag{6.2}$$

while the ARAP energy's Hessian was

$$\text{vec}\left(\frac{\partial^2 \Psi_{\text{ARAP}}}{\partial \mathbf{F}^2}\right) = 2\mathbf{I}_{9\times 9} - 2\mathbf{H}_1. \tag{6.3}$$

This is suspicious to say the *least*! Let's just come back to Earth and play a bit with that, it might reveal some clean structure for the eigenvalue as well. We already know the eigensystem of the rotation gradient:

$$\lambda_0 = \frac{2}{\sigma_x + \sigma_y} \qquad \mathbf{Q}_0 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{6.4}$$

$$\lambda_1 = \frac{2}{\sigma_y + \sigma_z} \qquad \mathbf{Q}_1 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}\mathbf{V}^T \tag{6.5}$$

$$\lambda_2 = \frac{2}{\sigma_x + \sigma_z} \qquad \mathbf{Q}_2 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{6.6}$$

We have $-2\mathbf{H}_1$, which just scales the eigenvalues of $\mathbf{H}_1$ by -2. Unfortunately, there is no magic theorem that would take the eigendecomposition of two matrices and then tell you the eigendecomposition of their sum...

Unless, if one of the matrices has a special structure, like $\mathbf{I}_{9\times 9}$! In that case, you can just add the eigenvalues from the diagonal matrix to the eigenvalues of your second matrix. The analytic eigendecomposition of the ARAP energy is then:

$$\lambda_0 = 2 - \frac{4}{\sigma_x + \sigma_y} \qquad \mathbf{Q}_0 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{6.7}$$

$$\lambda_1 = 2 - \frac{4}{\sigma_y + \sigma_z} \qquad \mathbf{Q}_1 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}\mathbf{V}^T \tag{6.8}$$

$$\lambda_2 = 2 - \frac{4}{\sigma_x + \sigma_z} \qquad \mathbf{Q}_2 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{6.9}$$

Back to the task we want to solve, how do we know if the energy goes indefinite? It's so easy now! E.g. for λ_0 it's

$$\begin{aligned} \lambda_0 = 2 - \frac{4}{\sigma_x + \sigma_y} &\leq 0, \\ 2 &\leq \frac{4}{\sigma_x + \sigma_y}, \\ \sigma_x + \sigma_y &\leq 2. \end{aligned} \tag{6.10}$$

and similarly $\lambda_{1,2}$ works out to

$$\lambda_1 \leq 0 \iff \sigma_y + \sigma_z \leq 2, \tag{6.11}$$

$$\lambda_1 \leq 0 \iff \sigma_x + \sigma_z \leq 2. \tag{6.12}$$

So basically what we need to do now in our simulator, is that if any of the conditions listed above in Eq. 6.10-6.12 are tripped over, that is, $\lambda_i \leq 0$, than make $\lambda_i = 0$.

With these analytical eigenvalues in hand, this becomes so straightforward, that I can explicitly list here how C++ doing this in the simulator:

```
virtual Mat9 ARAP::GetHessian(const Mat3& F) const override {

  // first calculate Σ, U, and V from the SVD of F and store the results
  JacobiSVD<Mat3> SVD{ F };
  const Vec3 Sigma = SVD.singularValues();
  const Mat3 U = SVD.matrixU();
  const Mat3 V = SVD.matrixV();

  double I[3]; // some precomputation
  I[0] = Sigma(0) + Sigma(1);
  I[1] = Sigma(1) + Sigma(2);
  I[2] = Sigma(0) + Sigma(2);
```

```
  // calculate the eigenvalues λ_i; clamp to 0.0 if necessary
  double lambda[3];
  for(int i = 0; i < 3; ++i)
    (I[i] >= 2.0) ? lambda[i] = 2.0 / I[i] : eigenvalue[i] = 1.0;

  // create the eigenmatrices Q_i = 1/√2 U T_i V^T from the twist matrices T_i
  Vec9 Q[3];
  for(int i = 0; i < 3; ++i)
    Q[i] = Flatten(sq2inv * U * T[i] * V.transpose());

  // build the hessian ∂²Ψ_ARAP/∂F² = 2I_9x9 − 2H_1
  Mat9 H = Mat9::Identity();
  for (int i = 0; i < 3; ++i)
      H -= lambda[i] * (Q[i] * Q[i].transpose());

  return 2.0 * H;

}
```

6.5 Analytical Eigendecompositions of Arbitrary Energies

Can we obtain such analytical eigendecomposition for *any* isotropic energy? Sure we can! We already have the eigenvalue of the first Smith et al. invariant, $\frac{\partial I_1}{\partial \mathbf{F}^2}$, that's what the previous section was all about. The eigensystem for $\frac{\partial I_2}{\partial \mathbf{F}^2}$ is also pretty easy, because it's a diagonal matrix.

The general eigensystem of I_3 is a bit more challenging. You can read the derivation in [15], Section 7.3. Actually I already reviewed the article which is all about that in the last paragraph of Sec. 6.3. It's basically doing the same thing what we did when we computed the rotation gradient.

Weirdly enough, $\lambda_{3\ldots5}$ and $\mathbf{Q}_{3\ldots5}$ is going to equal exactly $\lambda_{0\ldots2}$ and $\mathbf{Q}_{0\ldots2}$ from Eq. 6.7–6.9. $\lambda_{6\ldots8} = -\lambda_{3\ldots5}$ respectively, while the eigenmatrices $\mathbf{Q}_{6\ldots8}$ correspond to the *flip* eigenmode (instead of the *twist* eigenmodes of $\mathbf{Q}_{3\ldots5}$).

The first three eigensystem in the most general case, result in a quadratic system, that is encoded in a 3×3 matrix $\mathbf{A}$. We can construct this matrix $\mathbf{A}$ by probing $\frac{\partial^2 \Psi}{\partial \mathbf{F}}$ with scaling modes, e.g., the x-scaling vector is

$$\mathbf{D}_0 = \mathbf{U} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \mathbf{V}^T, \tag{6.13}$$

then the entries of $\mathbf{A}$ are obtained by computing the coefficients

$$a_{ij} = \operatorname{vec}(\mathbf{D}_i)^T \operatorname{vec}\left(\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}\right) \operatorname{vec}(\mathbf{D}_i)\,. \tag{6.14}$$

This might look a bit clumsy, but many popular distortion energies result in closed form expression for $\lambda_{0\ldots2}$, making them an excellent candidate for real-time use. They are listed in [25] Section 5, and [15] Section 7.3.4.

Chapter 7

Some Production Practicalities

Before jumping to the implementation details of the simulator, let's look at some smart tricks applied in the industry.

7.1 Geometric Calculation of the Deformation Gradient

First let's look at a new, clever – and I think a bit more intuitive – way to calculate the deformation gradient $\mathbf{F}$. The deformation gradient is the single most important measure in deformable simulation: it is the fundamental building block of all the calculation we have been doing. If you haven't done continuum mechanics before, you must be pretty excited to *finally* get your hands on the explicit formula for it.

7.1.1 The Mechanical Engineer's Way

Recall that we defined the motion which the structure is doing back in Sec. 4.1.2 as

$$\phi(\mathbf{x}) = \mathbf{F}\mathbf{x} + \mathbf{t} = \overline{\mathbf{x}}, \tag{7.1}$$

where $\mathbf{F}$ can be pretty much defined as

$$\mathbf{F} = \frac{\partial \overline{\mathbf{x}}}{\partial \mathbf{x}}. \tag{7.2}$$

We have a discretized structure in the form of a finite element mesh, which is a set of elements. An element is defined by some nodes. However, we are not talking about a set of particles, but a continuum instead, so what's up with that?

One way of thinking about this, is that we want a method to reconstruct a continuous deformation map from a set of discrete samples. It's pretty much a definition for an *interpolation scheme* – and this is the way to think about it in the mechanical engineers' finite element world. This means that each point $\mathbf{x}$ is defined as

$$\mathbf{x} = \sum_{i=1}^{n} h_i \mathbf{x}_i, \tag{7.3}$$

where h_i is a standard interpolation function – usually called *shape function* in this context – for an n noded element.

This is it! All you have to do now is to plug this definition of $\mathbf{x}$ to $\mathbf{F} = \frac{\partial \overline{\mathbf{x}}}{\partial \mathbf{x}}$, apply the chain rule, and you just aquired the deformation gradient for any element.

7.1.2 The Simulator Programmer's Way

Instead of plugging in Eq. 7.3 into the definition of $\mathbf{F}$, I'm going to present you a nice geometric way to calculate it. It was developed by Teran et al. in [12] and since its introduction, literally everybody discretizes deformables with this method in computer graphics. It defines 2D and 3D simplex elements (triangle and tetrahedron) with piecewise linear bases, with a single quadrature point in its center. E.g. in case of a 2D triangle, it basically ends up with what we would get, if we would plug in shape functions

$$h_0 = 1 - u - v, \qquad h_1 = u, \qquad h_2 = v, \tag{7.4}$$

into Eq. 7.3, then $\mathbf{F} = \frac{\partial \overline{\mathbf{x}}}{\partial \mathbf{x}}$, however, we will do it now in a much more intuitive way.

Calculating for a 2D Triangle

Let's say we have a triangle with vertices $\mathbf{x}_0$, $\mathbf{x}_1$, and $\mathbf{x}_2$. After deformation, these same vertices have become $\overline{\mathbf{x}}_0$, $\overline{\mathbf{x}}_1$, and $\overline{\mathbf{x}}_2$. The question now is how do we compute a $\mathfrak{R}^{2\times 2}$ matrix $\mathbf{F}$ that describes the rotation and scaling that occurs to transform the points $\overline{\mathbf{x}}_i$ into $\mathbf{x}_i$?

We definitely want to pull off any translations, so let's deal with that first. Both triangles are floating off in space somewhere, so just to establish a common point of reference, let's pull them both back to the origin. If they're centered about the origin, then no relative translation is needed to transform one into the other, and any remaining differences between the triangles must be due to rotation and scaling. We'll pull both triangles back to the origin by explicitly pinning $\overline{\mathbf{x}}_i$ and $\mathbf{x}_0$ to the origin (see Fig. 7.1).

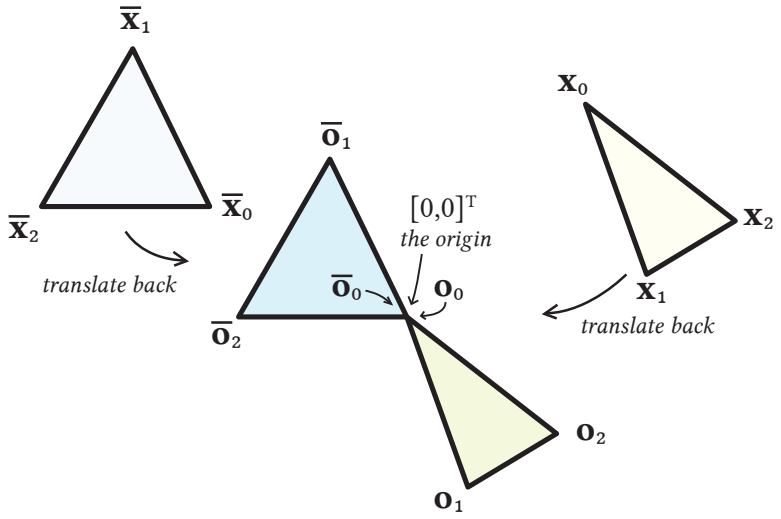


Figure 7.1: Let's eliminate the translation by pulling the *rest* triangle, back to the origin. We'll do the same thing to the *deformed* triangle as well.

The new vertices of our origin-centered rest-triangle become:

$$\begin{aligned} \mathbf{x}_0 &\rightarrow \mathbf{o}_0 = [0\ 0]^T, \\ \mathbf{x}_1 &\rightarrow \mathbf{o}_1 = \mathbf{x}_1 - \mathbf{x}_0, \\ \mathbf{x}_2 &\rightarrow \mathbf{o}_2 = \mathbf{x}_2 - \mathbf{x}_0. \end{aligned} \tag{7.5}$$

The vertices of the origin-centered deformed triangle are correspondingly:

$$\begin{aligned} \overline{\mathbf{x}}_0 &\rightarrow \overline{\mathbf{o}}_0 = [0\ 0]^T, \\ \overline{\mathbf{x}}_1 &\rightarrow \overline{\mathbf{o}}_1 = \overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_0, \\ \overline{\mathbf{x}}_2 &\rightarrow \overline{\mathbf{o}}_2 = \overline{\mathbf{x}}_2 - \overline{\mathbf{x}}_0. \end{aligned} \tag{7.6}$$

Now we want to know what matrix $\mathbf{F}$ will successfully rotate and scale all of our $\overline{\mathbf{o}}_i$ vertices so that they become the $\mathbf{o}_0$ vertices. In other words, we want the matrix $\mathbf{F}$ to satisfy these three equations:

$$\mathbf{F}\mathbf{o}_0 = \overline{\mathbf{o}}_0, \qquad \mathbf{F}\mathbf{o}_1 = \overline{\mathbf{o}}_1, \qquad \mathbf{F}\mathbf{o}_2 = \overline{\mathbf{o}}_2. \tag{7.7}$$

The first equation, $\mathbf{F}\mathbf{o}_0$ is trivially satisfied by any matrix $\mathbf{F}$, since both $\overline{\mathbf{o}}_0$ and $\mathbf{o}_0$ are all zeros. Really we only need to worry about $\mathbf{F}$ covering the other two cases by successfully producing $\overline{\mathbf{o}}_1$ and $\overline{\mathbf{o}}_2$ when provided with $\mathbf{o}_1$ and $\mathbf{o}_2$.
If we write this desire down explicitly, it's a well-posed linear algebra problem:

$$\begin{aligned} \mathbf{F}\left[\begin{array}{c|c} \mathbf{x}_1 - \mathbf{x}_0 & \mathbf{x}_2 - \mathbf{x}_0 \end{array}\right] &= \left[\begin{array}{c|c} \overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_0 & \overline{\mathbf{x}}_2 - \overline{\mathbf{x}}_0 \end{array}\right], \\ \mathbf{F}\left[\begin{array}{c|c} \mathbf{o}_1 & \mathbf{o}_2 \end{array}\right] &= \left[\begin{array}{c|c} \overline{\mathbf{o}}_1 & \overline{\mathbf{o}}_2 \end{array}\right], \\ \mathbf{F}\mathbf{D}_m &= \mathbf{D}_s. \end{aligned} \tag{7.8}$$

Computing the final $\mathbf{F}$ then becomes straightforward:

$$\boxed{\mathbf{F} = \mathbf{D}_s\mathbf{D}_m^{-1}.} \tag{7.9}$$

Calculating for 3D Tetrahedra

For a 3D tetrahedron, there is a straightforward generalization. In this case, we want a 3×3 version of $\mathbf{F}$. We translate the rest and the deformed versions to the origin again, and after observing that $\mathbf{F}\overline{\mathbf{o}}_0 = \mathbf{o}_0$ is again trivial, we are left with a 3×3 formulation:

$$\begin{aligned} \mathbf{F}\left[\begin{array}{c|c|c} \mathbf{x}_1 - \mathbf{x}_0 & \mathbf{x}_2 - \mathbf{x}_0 & \mathbf{x}_3 - \mathbf{x}_0 \end{array}\right] &= \left[\begin{array}{c|c|c} \overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_0 & \overline{\mathbf{x}}_2 - \overline{\mathbf{x}}_0 & \overline{\mathbf{x}}_3 - \overline{\mathbf{x}}_0 \end{array}\right], \\ \mathbf{F}\left[\begin{array}{c|c|c} \mathbf{o}_1 & \mathbf{o}_2 & \mathbf{o}_3 \end{array}\right] &= \left[\begin{array}{c|c|c} \overline{\mathbf{o}}_1 & \overline{\mathbf{o}}_2 & \overline{\mathbf{o}}_3 \end{array}\right], \\ \mathbf{F}\mathbf{D}_m &= \mathbf{D}_s, \\ \mathbf{F} &= \mathbf{D}_s\mathbf{D}_m^{-1}. \end{aligned} \tag{7.10}$$

Pretty cool, huh? Also, you can calculate the volume of the tetrahedron from

$$v = \frac{1}{6}|\det \mathbf{D}_m|. \tag{7.11}$$

7.1.3 Calculating the Derivative

Keeping up the momentum we also wanted the derivative

$$\frac{\partial \mathbf{F}}{\partial \mathbf{x}} = \frac{\partial \mathbf{D}_s}{\partial \mathbf{x}} \mathbf{D}_m^{-1}. \tag{7.12}$$

$\frac{\partial \mathbf{D}_s}{\partial \mathbf{x}}$ is a 3$^{\text{rd}}$-order tensor containing twelve matrices; as

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix} = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{11} \end{bmatrix}. \tag{7.13}$$

for a tetrahedra, the small matrices in the tensor (just as in Sec. 5.1) become

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{x}} = \begin{bmatrix} \begin{bmatrix} \frac{\partial \mathbf{D}_s}{\partial x_0} \end{bmatrix} \\ \begin{bmatrix} \frac{\partial \mathbf{D}_s}{\partial x_1} \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \frac{\partial \mathbf{D}_s}{\partial x_{11}} \end{bmatrix} \end{bmatrix}, \tag{7.14}$$

while $\mathbf{D}_m^{-1}$ is just a regular matrix. We get the result by multiplying through each $\frac{\partial \mathbf{F}}{\partial x_i} = \frac{\partial \mathbf{D}_s}{\partial x_i} \mathbf{D}_m^{-1}$. You can find the whole derivation in [15] Appendix E.

7.2 Force Computation Trick

This is nothing but a clever hack, and you probably already expect what it's all about, if you look at Fig. 7.2: consider the single quadrature point tetrahedra squished between your fingers. The force acting on the lower triangle ($\mathbf{f}_{1\ldots3}$) should sum up to be equal to the negative force acting on the top vertex ($-\mathbf{f}_0$), that is

$$\mathbf{f}_0 = -(\mathbf{f}_1 + \mathbf{f}_2 + \mathbf{f}_3). \tag{7.15}$$

We've just reduced the force computation from an $\mathfrak{R}^{12}$ to an $\mathfrak{R}^9$ problem. And you can do this with the force Jacobian as well:

$$\frac{\partial \mathbf{f}_i}{\partial \mathbf{x}_0} = -\left(\frac{\partial \mathbf{f}_i}{\partial \mathbf{x}_1} + \frac{\partial \mathbf{f}_i}{\partial \mathbf{x}_2} + \frac{\partial \mathbf{f}_i}{\partial \mathbf{x}_3} \right), \tag{7.16}$$

where we've reduced the $\mathfrak{R}^{12\times12}$ problem to an $\mathfrak{R}^{9\times12}$ by culling the first three rows of the Jacobian.

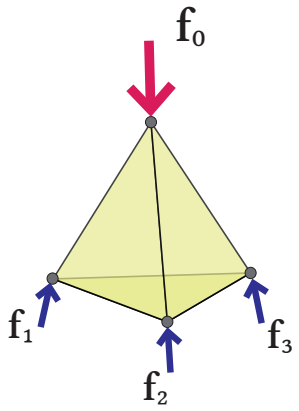


Figure 7.2: Optimizing force computation

7.3 Boundary Condition Projection

At any given step of a finite element simulation, a node is either completely unconstrained (though subject to forces), or the node may be constrained in either one, two or three dimensions.

The easiest way to introduce this concept to our simulator, is to simply delete the rows and columns corresponding to the constrained degrees of freedom from the final matrix. E.g. in case of the backward Euler formulation,

$$\left[\mathbf{M} - h\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}} - h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]\dot{\mathbf{u}} = h\mathbf{r} + h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\dot{\mathbf{x}}, \tag{7.17}$$

reduces to

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \tag{7.18}$$

and you just delete the corresponding rows and colums of $\mathbf{A}$.

This is completely fine, but I've found it really challenging to implement it efficiently. I instead implemented the mass modification constraint enforcement mechanics from the original Baraff-Witkin paper [2]. The idea of their method is pretty simple: it comes from an old-school hack applied in rigid-body dynamics simulators. Such dynamic simulators usually store the *inverse mass* of the particles: $\ddot{\mathbf{x}} = \frac{1}{m_i}\mathbf{f}_i$. When inverse mass is used, it becomes trivial to enforce constraints by altering the mass.

Suppose for example, that we want to keep particle i's velocity from changing. If we take $\frac{1}{m_i}$ to be zero, we give the particle an *infinite mass*, making it *ignore all forces exerted* on it. Complete control over a particle's acceleration is thus taken care of by storing a value of zero for the particle's inverse mass. What if we wish to constrain the particle's acceleration in only one or two dimensions? Although we'd normally think of a particle's mass as a scalar, we don't always need do so. Suppose that we write

$$\ddot{\mathbf{x}}_i = \begin{bmatrix} 1/m_i & 0 & 0 \\ 0 & 1/m_i & 0 \\ 0 & 0 & 0 \end{bmatrix}\mathbf{f}_i. \tag{7.19}$$

Now $\ddot{\mathbf{x}}_i$ must lie in the xy plane. Following this, an unconstrained particles inverse mass matrix is $\frac{1}{m_i}\mathbf{I}_{3\times 3}$.

Of course, we are not restricted to coordinate-aligned constraints. More generally speaking, given a unit vector $\hat{\mathbf{p}}_i \in \mathfrak{R}^3$, a particle is going to be prevented from accelerating along $\hat{\mathbf{p}}_i$ by using an inverse mass matrix $\frac{1}{m_i}(\mathbf{I} - \hat{\mathbf{p}}_i\hat{\mathbf{p}}_i{}^T)$. This comes from the fact that $(\mathbf{I} - \hat{\mathbf{p}}_i\hat{\mathbf{p}}_i{}^T)\hat{\mathbf{p}}_i = \mathbf{0}$. Similarly, given two mutually orthogonal unit vectors $\hat{\mathbf{p}}_i$ and $\hat{\mathbf{q}}_i$, we'd prevent a particle from accelerating in either the $\hat{\mathbf{p}}_i$ or $\hat{\mathbf{q}}_i$ direction by using the inverse mass matrix $\frac{1}{m_i}(\mathbf{I} - \hat{\mathbf{p}}_i\hat{\mathbf{p}}_i{}^T - \hat{\mathbf{q}}_i\hat{\mathbf{q}}_i{}^T)$. This trick really fascinates me! We've ended up with the filter $\mathbf{S}_i$ for each node, where

$$\mathbf{S}_i = \begin{cases} \mathbf{I}, & \text{if zero DOFs are constrained} \\ \mathbf{I} - \hat{\mathbf{p}}_i\hat{\mathbf{p}}_i{}^T, & \text{if one DOF } (\hat{\mathbf{p}}_i) \text{ is constrained} \\ \mathbf{I} - \hat{\mathbf{p}}_i\hat{\mathbf{p}}_i{}^T - \hat{\mathbf{q}}_i\hat{\mathbf{q}}_i{}^T, & \text{if two DOFs } (\hat{\mathbf{p}}_i \text{ and } \hat{\mathbf{q}}_i) \text{ are constrained} \\ \mathbf{0}, & \text{if all three DOFs are constrained} \end{cases} \tag{7.20}$$

then we modify $\mathbf{Ax} = \mathbf{b}$, according to [32] as

$$\left(\mathbf{SAS}^T + \mathbf{I} - \mathbf{S}\right)\mathbf{y} = \mathbf{Sc}, \tag{7.21}$$

$$\mathbf{y} = \mathbf{x} - \mathbf{z}, \tag{7.22}$$

$$\mathbf{c} = \mathbf{b} - \mathbf{Az}. \tag{7.23}$$

where $\mathbf{z}$ is the constrained vertices' velocity change.

This surely needs some explanation! The key equation is the first one. The $\mathbf{SAS}^T$ term is a straightforward projection of the original matrix $\mathbf{A}$ into the subspace spanned by the filters $\mathbf{S}$. According to Eberle in [15] (page 126) this creates a nearly rank-deficient matrix in the subspace comprised of the DOFs that were removed from the system. The $\mathbf{I} - \mathbf{S}$ term then *serves to improve the conditioning of this subspace.* Anywhere that filter was applied, the $\mathbf{I} - \mathbf{S}$ essentially gives things a boost with a bunch of ones.

This is the easiest to see if some particle i was constrained entirely, and $\mathbf{S}_i = 0$. Now we are in trouble because we have a 3×3 block of zeros along the diagonal. The *Gerschgorin circle theorem* (roughly) states that the eigenvalue corresponding to the row must lie inside some kind of disc. The diagonal entry prescribes the disc's center ($a_{ii} = 0$), and the radius is the absolute sum of the off-diagonal entries in that row ($r = \sum_{j\ j \neq i} \|a_{ij}\|$). The fact that the disc must be centered at zero is bad news, because it means that the eigenvalue is close to zero, and is almost certainly ruining the conditioning of the matrix. The $\mathbf{I} - \mathbf{S}_i$ fix will paste an identity matrix precisely on top of that zero block, and replace those zeros along the diagonal with ones. The Gerschgorin discs are now centered around one, and eigenvalues will be near one, which is a much better state.

7.4 Interpolating the Results on a Higher Resolution Mesh

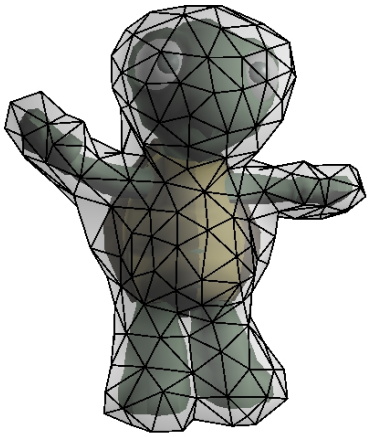


Figure 7.3: A high-res surface mesh embeded inside the volumetric FEM mesh.

In FEM, we simplify the structure to make the problem computable. However, we can easily interpolate the results on a higher resolution mesh, as you can see on Fig. 7.3.

First we need to figure out in which FEM element (e) each vertex of the higher resolution mesh $\hat{\mathbf{x}}_k$ is. Then we will calculate the $\hat{\mathbf{x}}_k$'s position, but in the FEM element's *local coordinate system*, that is, assigning an *interpolation weight* $\hat{h}_i$ – or more specifically a *barycentric weight* – to each FEM element vertex $\mathbf{x}_i^{(e)}$, so in the end we get back the original $\hat{\mathbf{x}}_k$ from

$$\hat{\mathbf{x}}_k = \sum_0^3 \hat{h}_i \mathbf{x}_i^{(e)}. \tag{7.24}$$

This is Eq. 7.3 for a 4-noded tetrahedron! You just calculate the weight $\hat{h}_i$ at startup or load them from disk, then the interpolation is nothing but this multiplication with the weight. So cheap!

Chapter 8

Implementing a Finite Element Simulator

As an example, what can be done with the nonsense I presented so far, I've implemented a *naive* simulator architecture. *Naive* here means, that I focused on readability and the educational value over performance, so it didn't become an interactive solution in the end. The full source code can be found at `marcisolti.github.io/ifem`. I used the following technologies for the implementation:

- The simulator is developed with **C++ on MSVC**.
- For all math related stuff – *'dense'* and *'sparse'* linear algebra, solution of sparse linear system with conjugate gradient, SVD – I used the **Eigen math library** [8]. This allowed me to translate the equations to C++ code almost in a 1:1 manner.
- **DirectX 12**[1] for drawing stuff on the screen real-time.
- Some naive parallelization is done with Intel's **Threading Building Blocks** (TBB)

[1]Special thanks for László Szécsi for the nice DirectX 12 class *(Grafikus játékok fejlesztése)* at BME-VIK.

8.1 Core Algorithm

First let me present you the *core algorithm* of our simulator. We will transform this algorithm to C++ code in a pretty straightforward manner. First we need to `initialize` the simulator where we precompute some stuff, then we will go to a `loop` where we timestep the chosen integrator forever:
`initialize` simulator:

- Parse config file
- Intialize the `EnergyFunction` class for computing $\frac{\partial \Psi}{\partial \mathbf{F}}$ and $\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}$.
- Load mesh, build mass matrix $\mathbf{M}$. (See Sec. 3.3.1)
- Parse boundary conditions, build $\mathbf{S}$. (Sec. 7.3)
- Precalculate $\mathbf{D}_m^{-1}$, v (as of Sec. 7.1.2) and $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ (Sec. 7.1.3) for each element.
- Setup the `Interpolator` class for calculating $\mathbf{f}_{ext}$.
- *(Set mesh initial position)*

`loop`:

1. T += dt,
2. According to config:
   (a) Get new $\mathbf{f}_{ext}$ from the `Interpolator`
   (b) *(Update* $\mathbf{S}$ *according to* $d\dot{\mathbf{u}}$*)*
3. Build $\mathbf{K}$ $\Rightarrow$ for each element:
   (a) Calculate $\mathbf{F} = \mathbf{D}_s \mathbf{D}_m^{-1}$ (As of Sec. 7.1.2)
   (b) Get the Jacobian $\frac{\partial \Psi}{\partial \mathbf{F}}$ from the `EnergyFunction` (Like in Sec 5.2.1)
   (c) $\mathbf{f}_{int}$ += $-v \frac{\partial \mathbf{F}}{\partial \mathbf{x}}^T \frac{\partial \Psi}{\partial \mathbf{F}}$ (See Eq. 5.5 and Eq. 5.18 in the beginning of Chapter 5.)
   (d) Get the Hessian $\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}$ from the `EnergyFunction`;
   either the Cauchy-Green way (Eq. 5.44) or the Smith et al. way (Eq 5.109)
   $\rightarrow$ add *'eigenvalues clamping'* if desired, according to Chapter 6.
   (e) Calculate $\frac{\partial^2 \Psi}{\partial \mathbf{x}^2} = -v \frac{\partial \mathbf{F}}{\partial \mathbf{x}} \frac{\partial^2 \Psi}{\partial \mathbf{F}^2} \frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ (See Eq. 5.38)
   (f) $\mathbf{K}$ += $\frac{\partial^2 \Psi}{\partial \mathbf{x}^2}$ according to Fig. 3.4.
4. **`do timestep`**
   See Sec. 8.2.6.

`endloop`

8.2 A Naive Simulator Architecture

We want to implement the core algorithm from Sec. 8.1 in C++ using the Eigen math library. As it's a *naive implementation*, focusing on readability and the code's educational value, we don't need to worry much about the architecture, so what about this:

```
// instantiate a solver object.
Solver solver;

// initialize the solver object with the config file
solver.StartUp(config)

// loop forever
while(1) {
  // step the simulation
  Vec result = solver.Step();

  // do whatever you want with the result
  // store it in memory, save it to disc, draw to the screen etc...
}
```

Seems pretty okay to me!

8.2.1 Configuring the Simulator

We want to tell tons of information to the simulator after the executable is built: what volumetric model to use, what are the material parameters, which are the loaded/constrained vertices; the list goes on. The most straightforward way would be a config file, more specifically a plain old `json` file. I used the classic C++ json implementation by Niel Lohmann [17]. An example for the data structure is listed in Appendix C.

8.2.2 The Solver Class

In Sec. 8.2 I showed how the simulator should be used: We instantiate a `Solver` object – like `Solver solver` – then we call this instance's methods – as `solver.StartUp(config)` or `solver.Step()` – in order to do something with it.

This is because I used the object-oriented programming paradigm, where the data and their methods to manipulate it are grouped together in the form of objects. We define a **`class`** or a prototype of an object, then we instantiante these prototypes. Intuitively, a **`class`** is a cookie cutter, while it's instance is the cookie you cut with the cookie cutter from the dough.

So our main goal is to define a class which can be used in the way we determined in Sec. 8.2. I did this:

```
class Solver
{
  // some resources for the simulator
  // presented in the next section

public:
  // methods for initialization/deinitialization
  Vec StartUp(json* config);
  void ShutDown();

  // stepping the simulator
  Vec Step();

  // helper functions
private:
  void BuildFintAndKeff();
  void ComputeElementJacobianAndHessian(int i);

  void FillFint();
  void FillKeff();

  Mat3  ComputeDm(int i);
  Mat9x12 ComputedFdx(Mat3 DmInv);
};
```

8.2.3 Resources

We have our methods defined, what about the data? Let me walk you through the data fields of the solver class, which lays out all the necessary resources for a FEM simulator. The first thing is an enumeration defined outside the solver class

```
enum Integrator { qStatic, bwEuler, Newmark };
```

which is nothing but a more convinient way to say

```
int integrator = ...; // 0 = qStatic, 1 = bwEuler, 2 = Newmark
```

Our `Solver` class look like this:

```
class Solver
{
  json* config;

  VolumetricMesh* mesh;
  uint32_t numDOFs, numElements, numVertices;
  std::vector<int> indexArray;

  Integrator integrator;
  EnergyFunction* energyFunction;

  // time integration variables
  double T, h, magicConstant;
  uint32_t numSubsteps;
  double alpha, beta;

  // boundary conditions
  Interpolator interpolator;
  std::vector<int> loadedVerts, BCs;
  SpMat S;
```

```
  // matrices and vectors
  SpMat Keff, M, spI;
  Vec x_0, u, x, v, a, z, fExt;

  // precomputed stuff
  std::vector<double> tetVols;
  std::vector<Mat3> DmInvs;
  std::vector<Mat9x12> dFdxs;

  // linear solver object
  ConjugateGradient cgSolver;

public:
  // methods presented before
};
```

First we have the `json* config`, which stores a pointer – a reference – to the global `config` object. The app's whole state is stored in a `json` object, which allows me to easily serialize/deserialize – load from/save to the disc – the whole app's state.

We then have a `VolumetricMesh* mesh`, which stores a pointer – not so supprisingly – to the volumetric mesh. I used the Vega FEM library's [3] volumetric mesh class, which allows me to load meshes from disk in their proprietary `.veg` format.

There's not too much about it: it's nothing but a text file, containing a list of vertices and a list of vertex indices, defining volumetric mesh data. In the not so distant future I would like to define my own mesh interface, as I'm planning to support mesh import from *'proper'* FEM softwares – e.g. ANSYS, or my personal favourite, Hypermesh.

`uint32_t numDOFs, numElements, numVertices;` is storing the number of DOFs, etc., in a 32-bit wide unsigned integer, or in other words, in a regular integer but without the sign. In the `std::vector<int> indexArray` I store the index of each tetrahedron: as tetrahedra has 4 vertices, each 4 `int` makes up a tetrahedron, so the `vector`'s length is `4 * numElements`.

The `integrator` is nothing but a glorified `int` as we've discussed it previously. `energyFunction` is a pointer to an `EnergyFunction` object. We will discuss this in the next section.

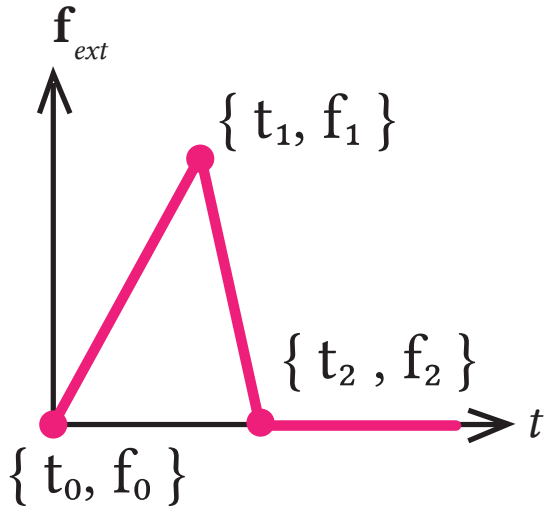
The next set of numbers – `double` is a double precision floating point a.k.a. real number – are some time integration variables. The time integration methods are presented in Sec. 8.2.6.

The `interpolator` object stores the load steps and interpolates between them with simple linear interpolation: you get the value for f in case of a specific t from

$$f = f_i + (t - t_i)\frac{f_{i+1} - f_i}{t_{i+1} - t_i}. \tag{8.1}$$

You define your load steps in the `json` as you can see on Fig. 8.1. Then you just call `interpolator.get(t)` and you get your $\mathbf{f}_{ext}$ value for a specific timepoint t.

We store a list of integers – a.k.a. `std::vector<int>` – for both the loaded and fixed vertex indices. We also have the sparse matrix object – `SpMat` – for the matrix $\mathbf{S}$, as of Sec 7.3. Next up are all the sparse resources for time integration, like $\mathbf{K}$, $\mathbf{M}$, or $\mathbf{f}_{int}$ and $\mathbf{f}_{ext}$, etc., we will use these extensively in Sec. 8.2.6.




```
"loadSteps": [
  {
    "f": 0.0,
    "t": 0.0
  },
  {
    "f": 10000.0,
    "t": 5.0
  },
  {
    "f": 0.0,
    "t": 6.0
  },
  ...
],
```

Figure 8.1: Linear interpolation for the load steps

It is a significant optimization to precalculate stuff, and we are able to do that with $\mathbf{D}_m^{-1}$, v, and $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ for each element. These are stored in the `vectors` `DmInvs`, `tetVols` and `dFdxs` respectively.

Last but definitely not least, we have our conjugate gradient solver object `cgSolver`, provided by Eigen to us.

8.2.4 Initialization

Before we can *finally* start using our simulator, we need to do some precalculations and initialization at the application startup. This was pretty much written down already in the core algorithm (Sec. 8.1), the only part that needs some further explanation is the initialization of the `EnergyFunction`.

Yet another principle of object-oriented programming coming up: different `EnergyFunction` classes are *derived* from the `EnergyFunction` base class, thus all descended `EnergyFunction` classes inherit all the data and member function of the base class. That is one feature of the derived classes, another one is polymorphism: we can use different classes with the same interface:

```
// two EnergyFunction pointers
EnergyFunction* arap, neoHookean;

// create the ARAP and NeoHookean instances
// both are derived from the EnergyFunction class
// so you can use EnergyFunction* pointers to reference them
arap = new ARAP{ E1, nu1 };
neoHookean = new NeoHookean{ E2, nu2 };

// GetJacobian(const Mat3& F) is a method of the base class
// So you can call it from any of the derived classes
// This means that you use all the derived energy function classes the same way
Vec9 arapJacobian = arap->GetJacobian(F);
Vec9 neoHookeanJacobian = neoHookean->GetJacobian(F);
```

This will come in handy in the simulation loop! But for now, at initialization, our duty is to figure out which `EnergyFunction` we want to use. This is done by parsing the config file and calling a good ole' **new** on the corresponding energy function.

```
if (energyName == "ARAP") {
  energyFunction = new ARAP{ E, nu };
} else if(energyName == "SNH")
  energyFunction = new StableNeoHookean{ E, nu };
} else if(energyName == "StVK")
  energyFunction = new StVK{ E, nu };
}
```

These are the `EnergyFunctions` supported by the simulator:

- Projected ARAP as of Sec. 6.4,
- classic Saint Venant-Kirchhoff,
- or Smith et al. Stable Neo-Hookean from [24].

Next up, is to deal with a practical thing: we've initialized the `EnergyFunction` with `E` and `nu`, which is not `mu` and `lambda` we were talking about all the time. μ and λ are the *Lamé parameters*, which are perfectly fine, however, Young's modulus E and Poissons's ratio ν are much more common. If you look up a real material's data, it's probably going to be $\{E, \nu\}$ not $\{\mu, \lambda\}$, so I made $\{E, \nu\}$ the default. $\{\mu, \lambda\}$ are calculated at initialization from

$$\mu = \frac{E}{2(1+\nu)}, \tag{8.2}$$

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}. \tag{8.3}$$

We also precompute some other stuff necessary for each `EnergyFunction`, e.g. all the fixed $\mathbf{T}_i$ twist matrices for ARAP, $\frac{1}{\sqrt{2}}$ as `1.0/std::sqrt(2.0)`, etc.

8.2.5 Simulation loop

After we initialized everything, we'll get into an infinite loop

```
while(1) {
  Vec result = solver.Step();
  // do stuff with the result ...
}
```

stepping the simulation forward forever in time.
Each timestep starts with some setup:

1. Set stuff: `int subStep = 0; T += h;`
2. Get the load value $\mathbf{f}_{ext}$ from the `interpolator`:
   `double loadValue = interpolator.get(T)`
3. Set $\mathbf{f}_{ext}$ according to the config and the `interpolator`:
   `for (auto index : loadedVerts) fExt(index)  = loadValue;`
4. Zero $\mathbf{f}_{int}$ and $\mathbf{K}$

Then the magic is happening here:

```
for(;;) // loop forever
{
  // Build f_int and K
  BuildFintAndKeff();

  // do a timestep according to the chosen integrator
  switch(integrator)
  {
    case qStatic:
    {
      // do timestep the quasistatic way ...
    }
    break;
    case bwEuler:
    {
      // do timestep the backward Euler way ...
    }
    break;
    case Newmark:
    {
      // do timestep the Newmark way ...
    }
    break;
  }

  // exit the loop if you did sufficient amount of substeps
  if(++substep >= numSubsteps)
      break;
}
```

I think this code is pretty self-explanatory: we build $\mathbf{f}_{int}$ and $\mathbf{K}$, then do a timestep with the chosen integrator scheme. But what schemes are available, exactly?

8.2.6 Time Integration

Back in Sec. 3.3.2 we looked at ways how to timestep a *dynamic process*, and arrived at the closed form solution for $\dot{\mathbf{u}}$. But what about just simply timestepping the plain old $\mathbf{Ku} = \mathbf{f}$ first, does that make sense?

Quasistatic Formulation

Yes it does, and it's called the *quasistatic formulation*. It's basically the regular Newton-Raphson iteration from Sec. 3.2.3:

$$\mathbf{Ku} = -\mathbf{f}_{int} + \mathbf{f}_{ext}, \tag{8.4}$$

$$\mathbf{x} \mathrel{+}= \kappa\mathbf{u}. \tag{8.5}$$

where κ is specified with line search in [25], but you can find the process in the Bonet-Wood book [6] as well (Section 9.6.2). I didn't want to implement a line search *yet*, so I used a magic constant instead which has to be sufficiently small. This was implemented in the simulator in the following way:

```
case qStatic:
{
  // Ku = -f_int + f_ext
  // then do the constraint projection stuff
  SpMat SystemMatrix = S * Keff * S + spI - S;
  Vec SystemVec = S * (-fInt + fExt);

  // factorize and solve the final matrix
  solver.compute(SystemMatrix);
  Vec u = solver.solve(SystemVec);

  // increment as x += κu
  x += magicConstant * u;
}
break;
```

Isn't it nice to see how clearly math translates to C++?

Dynamics Simulations

We've derived the **backward Euler** timestepping scheme back in Sec. 3.3.2, which is

$$\left[\mathbf{M} - h\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}} - h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]\dot{\mathbf{u}} = h\mathbf{f} + h^2\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\dot{\mathbf{x}}; \tag{8.6}$$

$$\dot{\mathbf{x}} \mathrel{+}= \dot{\mathbf{u}}, \tag{8.7}$$

$$\mathbf{x} \mathrel{+}= h\dot{\mathbf{x}}. \tag{8.8}$$

It translates to C++ pretty well too:

```
case bwEuler:
{
  //h(f_int + f_ext) + h^2 ∂f/∂x ẋ
  Vec RHS = h * ((fInt + fExt) + h * Keff * v);

  //[M - h ∂f/∂ẋ - h^2 ∂f/∂x]
  SpMat EffectiveMatrix = M - h * (alpha * Keff + beta * M) - h2 * Keff;

  // project constaints
  Vec SystemVec = S * RHS;
  SpMat SystemMatrix = S * EffectiveMatrix * S + spI - S;


  solver.compute(SystemMatrix);
  Vec dv = solver.solve(SystemVec);

  v += dv;
  x += h * v;
}
break;
```

So easy! I also implemented the **implicit Newmark** scheme, because why wouldn't I do it, I just had to look it up in the university FEM lecture notes [31]. In case of constant acceleration, $\alpha = 1/4$, and $\gamma = 1/2$, so the Newmark scheme becomes:

$$\left(\frac{4\mathbf{M}}{h^2} + \frac{2\mathbf{C}}{h} + \mathbf{K}\right)\mathbf{u}_{i+1} = \mathbf{f}_{i+1} + \mathbf{M}\left(\ddot{\mathbf{u}}_i + \frac{4}{h}\dot{\mathbf{u}}_i + \frac{4}{h^2}\mathbf{u}_i\right) + \mathbf{C}\left(\dot{\mathbf{u}}_i + \frac{2}{h}\mathbf{u}_i\right); \tag{8.9}$$

$$\dot{u}_{i+1} = \frac{2}{h}\left(\mathbf{u}_{i+1} - \mathbf{u}_i\right), \tag{8.10}$$

$$\ddot{u}_{i+1} = \frac{4}{h^2}\left(\mathbf{u}_{i+1} - \mathbf{u}_i\right) - \frac{4}{h}\dot{\mathbf{u}}_i - \ddot{\mathbf{u}}_i. \tag{8.11}$$

I omitted the C++ but it's the same straightforward translation as before.

8.2.7 Building The Force Jacobian

After 75 pages of blood and sweat, we arrived at the C++ listing of the force Jacobian calculation. In Sec. 8.2.5, we called the function `BuildFintAndKeff()`:

```
void Solver::BuildFintAndKeff()
{
  for(int i = 0; i < numElements; ++i)
    ComputeElementJacobianAndHessian(i)
}
```

`ComputeElementJacobianAndHessian(i)` then calculates $\mathbf{f}_{int}$ and $\mathbf{K}$ for the i^{th} element. According to the core algorithm from Sec. 8.1, it was something like this:

1. Calculate $\mathbf{F} = \mathbf{D}_s\mathbf{D}_m^{-1}$ (As of Sec. 7.1.2)
2. Get the Jacobian $\frac{\partial\Psi}{\partial\mathbf{F}}$ from the `EnergyFunction` (Like in Sec 5.2.1)
3. $\mathbf{f}_{int}$ += $-v\frac{\partial\mathbf{F}}{\partial\mathbf{x}}^T\frac{\partial\Psi}{\partial\mathbf{F}}$ (See Eq. 5.5 and Eq. 5.18 in the beginning of Chapter 5.)
4. Get the Hessian $\frac{\partial^2\Psi}{\partial\mathbf{F}^2}$ from the `EnergyFunction`
5. Calculate $\frac{\partial^2\Psi}{\partial\mathbf{x}^2} = -v\frac{\partial\mathbf{F}}{\partial\mathbf{x}}\frac{\partial^2\Psi}{\partial\mathbf{F}^2}\frac{\partial\mathbf{F}}{\partial\mathbf{x}}$ (See Eq. 5.38)
6. $\mathbf{K}$ += $\frac{\partial^2\Psi}{\partial\mathbf{x}^2}$ according to Fig. 3.4.

Let me just walk you through the explicit C++ from the simulator! We'll start by getting the 4 indices for the vertices we are going to work with, then calculate the deformation gradient $\mathbf{F}$ following Sec. 7.1.2.

```
void Solver::ComputeElementJacobianAndHessian(int i)
{
  const int* indices = &(indexArray[4 * i]); //← not pretty ...
```

```
Mat3 F;
{
  Vec3 v0, v1, v2, v3; // filling up vectors with the << operator
  {
    v0 << x(indices[0] + 0), x(indices[0] + 1), x(indices[0] + 2);
    v1 << x(indices[1] + 0), x(indices[1] + 1), x(indices[1] + 2);
    v2 << x(indices[2] + 0), x(indices[2] + 1), x(indices[2] + 2);
    v3 << x(indices[3] + 0), x(indices[3] + 1), x(indices[3] + 2);
  }

  const Vec3 ds1 = v1 - v0;
  const Vec3 ds2 = v2 - v0;
  const Vec3 ds3 = v3 - v0;

  // you can use << to fill up matrices as well.
  Mat3 Ds;
  Ds <<
    ds1[0], ds2[0], ds3[0],
    ds1[1], ds2[1], ds3[1],
    ds1[2], ds2[2], ds3[2];
  const Mat3 DmInv = DmInvs[i];
  F = Ds * DmInv;
}
```

That's it! We have discritized the kinematics! Loving this method for calculating $\mathbf{F}$! Next up: calculating $\mathbf{f}_{int}$ the the i^{th} element:

```
// get v
const double tetVol = tetVols[i];
// get the precomputed vec(∂F/∂x)
const Mat9x12 dFdx = dFdxs[i];
{
  // and the Jacobian vec(P) = vec(∂Ψ/∂F)
  const Vec9 Pv = energyFunction->GetJacobian(F);

  // the internal forces then are nothing but
  // f_int^(i) = -v vec(∂F/∂x)^T vec(∂Ψ/∂F)
  const Vec12 fEl = -tetVol * dFdx.transpose() * Pv;

  // then add f_int^(i) to the global f_int
  for (int el = 0; el < 4; ++el)
    for (int incr = 0; incr < 3; ++incr)
      fInt(indices[el] + incr) += fEl(3 * el + incr);
}
```

Yet again a straightforward transformation of math to C++! The Jacobian can be constructed in the same manner:

```
{
  // get vec(∂²Ψ/∂F²)
  const Mat9 dPdF = energyFunction->GetHessian(F);

  // we already have the precomputed vec(∂F/∂x), so the Hessian is
  // K^(i) = -v vec(∂F/∂x)^T vec(∂²Ψ/∂F²) vec(∂F/∂x)
  const Mat12 dPdx = -tetVol * dFdx.transpose() * dPdF * dFdx;
```

```
    // now we just add K^(i) to the global K with this crazy loop
    for (int y = 0; y < 4; ++y)
      for (int x = 0; x < 4; ++x)
        for (int innerY = 0; innerY < 3; ++innerY)
          for (int innerX = 0; innerX < 3; ++innerX)
            Keff.coeffRef(indices[x] + innerX, indices[y] + innerY) +=
            dPdx(3 * x + innerX, 3 * y + innerY);

  }
}
```

Except for that crazy loop at the end, it wasn't that hard either right? And we are just done! We finally have this mighty force Jacobian defined. However, this code is a bit slow, and we can tweak it a tiny bit to make it much-much faster with some trivial trickery.

8.2.8 Naive Parallelization of the Global Matrix Assembly

Did you know that computers now have more CPUs inside their CPU? It's crazy, right? The whole thing is called CPU, while the CPUs inside the CPU are called *cores*. E.g. if you have a CPU with 4 cores, you can run 4 streams of machine language instructions in parallel. In other words, instead of executing 1 instruction per cycle, you can execute 4! It's not that simple, but this is the core idea.

So we have this big $\mathbf{K}$ and $\mathbf{f}_{int}$ calculation loop, which we do *for each element*. This sounds like an excellent example for parallel programming! E.g. if you have 1000 elements, instead of calculating all 1000 of them on a single core, you can divide it up between the cores, e.g. do 250 on each core parallel, if you have 4 of them.

However, the $\mathbf{K}$ and $\mathbf{f}_{int}$ calculation is not trivially parallelizable yet: the process of adding the element forces $\mathbf{f}_{int}^{(i)}$ and stiffness matrices $\mathbf{K}^{(i)}$ to the global vector/matrix can cause some trouble. More specifically, we can do some nonsense if we want to add to *the same element in the same time* in the global matrix/vector.

The trivial solution to this problem would be to collect the element forces $\mathbf{f}_{int}^{(i)}$ and stiffness matrices $\mathbf{K}^{(i)}$ in an array, storing a $\mathfrak{R}^{12}$ vector and a $\mathfrak{R}^{12\times12}$ matrix for each element. Doesn't sound that complicated, right? The process is visualized on Fig. 8.2. Then in the second step, we add these element forces/stiffness matrices to the final, global system.

First we need to add these new arrays to the `Solver` class:

```
class Solver {
  // ...
  // parallel Keff building resources
  std::vector<Vec12>  fIntArray;
  std::vector<Mat12>  KelArray;
};
```

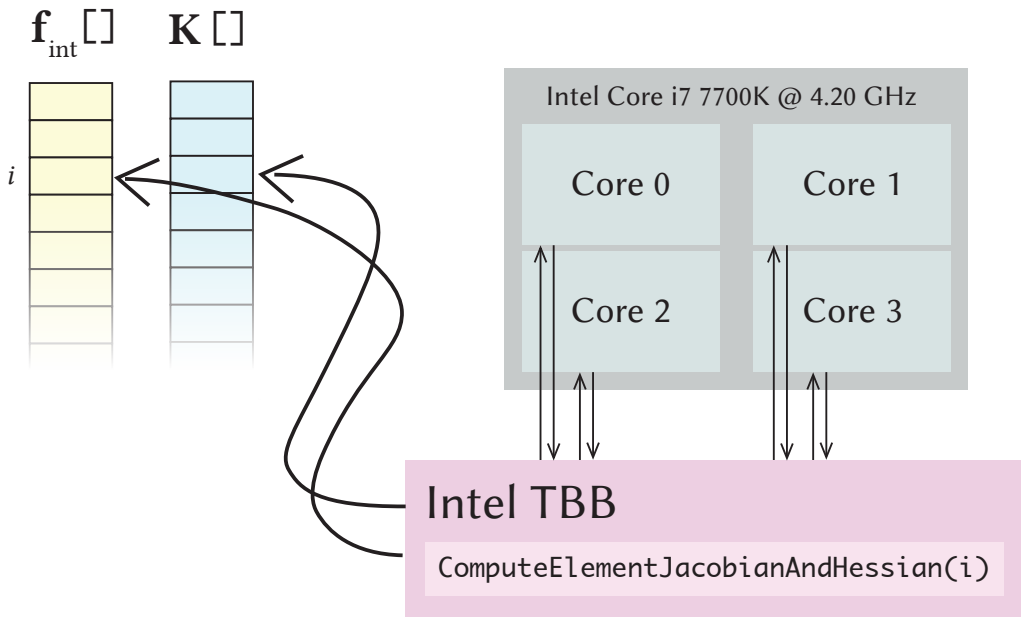


Figure 8.2: Naive parallelization of building $\mathbf{f}_{int}$ and $\mathbf{K}$

Then the method `ComputeElementJacobianAndHessian(i)` is modified as:

```
Solver::ComputeElementJacobianAndHessian(int i)
{
  // calculate F ...

  {
    // ...
    // calculate forces ...
    const Vec12 fEl = -tetVol * dFdx.transpose() * Pv;

    // instead of adding directly to the global f_int,
    // we assign it to the appropriate array element
    fIntArray[i] = fEl;
  }

  {
    // ...
    // get Jacobian
    const Mat12 dPdx = -tetVol * dFdx.transpose() * dPdF * dFdx;

    // do the same with K
    KelArray[i] = dPdx;
  }
}
```

Then in the `Step()` method, we just replace the regular `for` with a `tbb::parallel_for`, provided by Intel's Threading Building Blocks interface (TBB). Yes, it's that easy – since we made the problem trivially parallelizable.

```
Vec Solver::Step()
{
  // setup ...
  for(;;)
  {
    tbb::parallel_for(
      tbb::blocked_range<size_t>(0, numElements),
      [=](const tbb::blocked_range<size_t>& r)
      {
        for (size_t i = r.begin(); i != r.end(); ++i)
          ComputeElementJacobianAndHessian(i);
      }
    );
    // ...
```

Then we just need to accumulate the content of the $\mathbf{f}_{int}^{(i)}$ and $\mathbf{K}^{(i)}$ vectors

```
FillFint();
FillKeff();
```

How much faster is this? E.g. in the turtle example (see Sec. 9.1 – it's 1185 elements) the assembling the global matrix/vector took ~0.38 s without parallelization, while the parallelized version took ~0.1 s. Wow! That's a ~3.8x performance increase with a small tweak! I love technology!

8.3 Drawing the Results On The Screen

Calling the `Step()` method is going to return $\mathbf{x}$, the current position of all the vertices. If a step would take less than 1/60s = 0.0167 s we could animate the model in real-time, but this is not the case unfortunately. Even Eigen's conjugate gradient routine of e.g. the turtle example's (Sec. 9.1) ~1000 × 1000 matrix takes about 0.05 s, so we would need a significantly different application for that.

Let's just cook from what we have. In my opinion, a 0.15s long timestep is not that bad, so the application I built around this solver accumulates all the $\mathbf{x}$s in a `vector`, and we can *'play'* this – using an industry term – *'baked'* animation.

8.3.1 A Basic Real-Time Graphics Application

We have this `std::vector<x> positionArray`, how to draw it to the screen? Probably DirectX 12 is not the best solution for this, because it's a low-level graphics API, and we have to do stuff which may seem unnecessary, but I have a little engine written in DirectX already, so I just used that. We again have to do the same things we did with the solver. First we initialize the app, then define what should be done when a frame is drawn. **`initialization`** looks like this:

- Open window
- Parse config
- Start subsystems: `App`, `Renderer` and `Simulator`.

The `App` provides us a lil' GUI (`ImGui`), where we can manipulate stuff about the app, e.g. choose the frame we want to display. We then start the `Simulator` system. It is basically a thin wrapper around a `Solver` instance, which prepares the model for display and posesses the array of the resultant **x**s.

The `Renderer` does the rendering. In Sec. 2.1 I talked a bit about what you need to render stuff. On initialization, the `Renderer` creates and uploads some resources on the GPU:

- Geometry: mesh defined by a list of vertices and a list of triangles.
  Data at each vertex: position, *normal*, UV coordinates, etc.
- Texture(s): *Per-pixel* color – or any other – data mapped on the triangles
- Constant Buffer(s): *Per-object*, global data. E.g. model's position, rotation, etc.
- Shader(s): GPU code for shading each object
- Abstract resources for shading: camera and light sources

We push all this stuff on the GPU on startup.

As I said our solver is *not* running at 60 fps, but around 6-7 fps. To be able to pleasantly move around the model, we need to step a simulation on a separate thread, while the main rendering loop just displays the result. Stepping the simulation on a separate thread looks like this:

```
void Simulator::Step() {
  // the simulator class calls the solver's method to do a timestep
  Vec currentPosition = solver.Step();
  // and stores the result
  positionArray.push_back(currPos);
  stepNum++;
}

void StepSimulator() {
  // The Simulator is running on a separate thread forever
  // not bothering with any of the app/rendering stuff going on
  while(1) {
    sim.Step();
  }
}

// in main():
// creating the thread
std::thread simThread{ StepSimulator }
```

Now the **`main loop`** looks like this:

- Update the App's state
- Update the Simulator.
  For the currently selected time step:
  1. Get mesh vertices
  2. Recalculate normals
  3. Upload mesh
- Draw Scene

What is up with that normal recalculation tough?

8.3.2 Drawing the Model

To color the triangle we need to integrate the rendering equation [13]. There are smart ways to do that, but I'm not going to talk about it, as this thesis is already far too long. If you're interested, the best thing you can do is checking out the BME BSc lecture on Computer Graphics.

What we are essentially doing is visualized on Fig. 8.3. We simulate the light's interaction with a surface. What's important now is you need the position and the *normal vector* of the surface in order to determine its color. We've just written a huge application which will determine the position of a deformed surface, but what about the normal vector? We'll need to compute the normal vector at each vertex for each time a frame is drawn. There is a nice trick to this that I want to show you now.

Triangle Mesh Normal Vector Calculation Hack

This is really just a hack: first, initialize an array of 3 component vectors to zero for each triangle vertex. Then, for each triangle, calculate the normal vector of the triangle

$$\mathbf{n}_i = (\mathbf{b} - \mathbf{a}) \times (\mathbf{c} - \mathbf{a}), \tag{8.12}$$

then calculate the triangle area

$$A_i = \frac{1}{2}\|\mathbf{n}_i\|, \tag{8.13}$$

then *'normalize'* it with its area, so bigger triangles count more:

$$\mathbf{n}_i \mathrel{*}= \frac{1}{2A_i}, \tag{8.14}$$

then add this normal $\mathbf{n}_i$ to each vertex the triangle is *'made of'*. You will end up with a nice approximation of the surface normals at the vertices. See Fig. 8.4 for visualization.

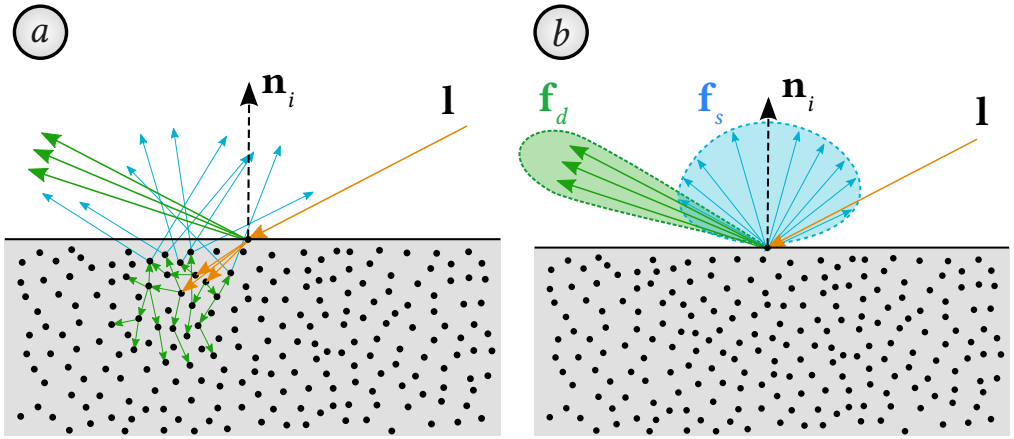


Figure 8.3: a – Photons interacting with a surface. b – Model applied in rendering [22].

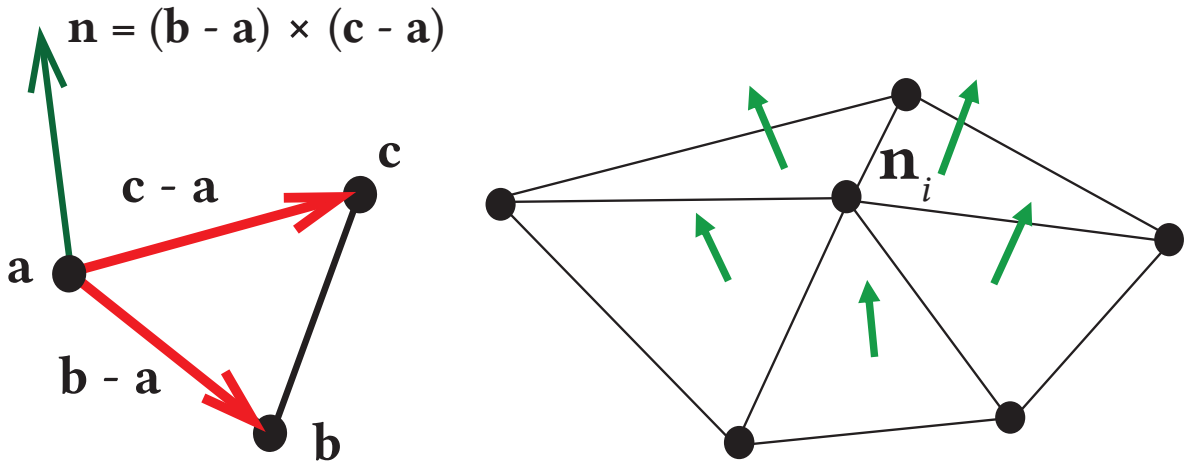


Figure 8.4: Computation of the normal vector.

Chapter 9

Case Studies

9.1 Testing Rig, Example Models

Let's try our brand new simulator! The rig I used for the simulation is an avarage gaming PC from early 2017: 14 nm, quad core, hyperthreaded Intel 7700K running at 4.20 GHz. The cooling solution was cleaned a long-long time ago, which might contribute to the result. The simulator is a fully CPU side app, so the GPU doesn't matter, but it was a GeForce 1060 3GB.

I used 3 volumetric mesh examples from the Vega FEM library [4]: the 'turtle', (Fig. 9.1a) the *'cantilever plate'*, (Fig. 9.1b), the 'asian dragon' (Fig. 9.1c) and the 'simple bridge' (Fig. 9.1d). You can see the fixed and the loaded vertices on Fig. 9.1. For all the simulations, I applied some force incrementally with the `Interpolator` class till a specified $\mathbf{f}_{max}$, then I sort of *'released'* it, just like in the loading situtation on Fig. 8.1.

9.2 Testing the Core Algorithm

Believe it or not, the simulator presented in the previous chapter... works! You can either go down the Cauchy-Green way (Eq. 5.44) or the Smith et al. way (Eq 5.109), you just need to derive the scalar derivative of any `EnergyFunction` you find in the literature. However, without the Hessian projection, as of Chapter 6, you need some sufficiently small timesteps.

I tested the core algorithm on the *Saint Venant-Kirchhoff*, *Stable Neo-Hookean* [24] and of course on the *ARAP* material models. You can see the results on Fig. 9.1a and b. All of them worked pretty well, with *sufficiently small timesteps*.

9.3 Projected Newton Solver

With the analytical eigensystem of the ARAP energy, presented in Sec. 6.4, we can easily implement the projected Newton solver from [25]. Does it work? **drumrolls** It does!

As you can see on Fig. 9.2a and b, crushing the asian dragon or the turtle model to a plane doesn't cause the simulation to explode, it rather successfully recovers to its rest state. On the other hand, if you delete the lines doing the *Hessian projection*, the simulation *does* explode. I consider this an *epic win*.

9.4 Dynamics Simulations: What?

This is definitely the peak of my sloppiness in this thesis, but I just can't figure out what – *if anything* – is wrong with the dynamic integration of my solver. First, I definitely should've paid more attention to the amazing vibration and dynamics lectures at the university. That's probably the biggest mistake.

The issue I have is that compared the quasistatic case (Sec. 8.2.6), dynamic integration with implicit Newmark or backward Euler seems infinitely less stable to me. It sounds okay when I write this down but shouldn't implicit integration allow larger timesteps? It allowed *way larger* timesteps than the explicit method I tried, but compared to the same time integration in the Vega FEM library, it was $10 - 1000$ times slower. Weird! Although with sufficiently small timesteps, it worked, which is nice. And surprisingly, the backward Euler seemed a bit more stable for me.

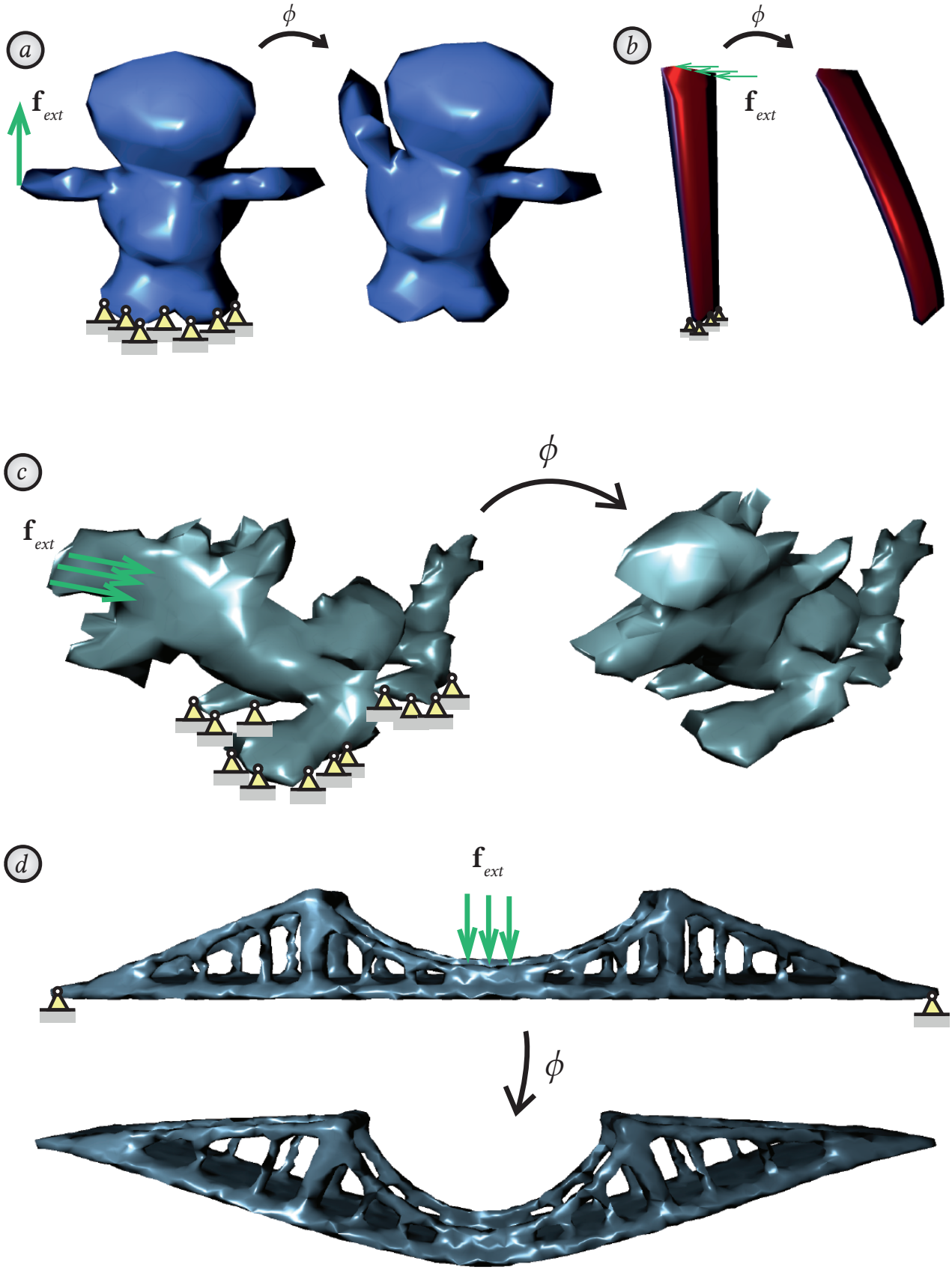


Figure 9.1: Results.

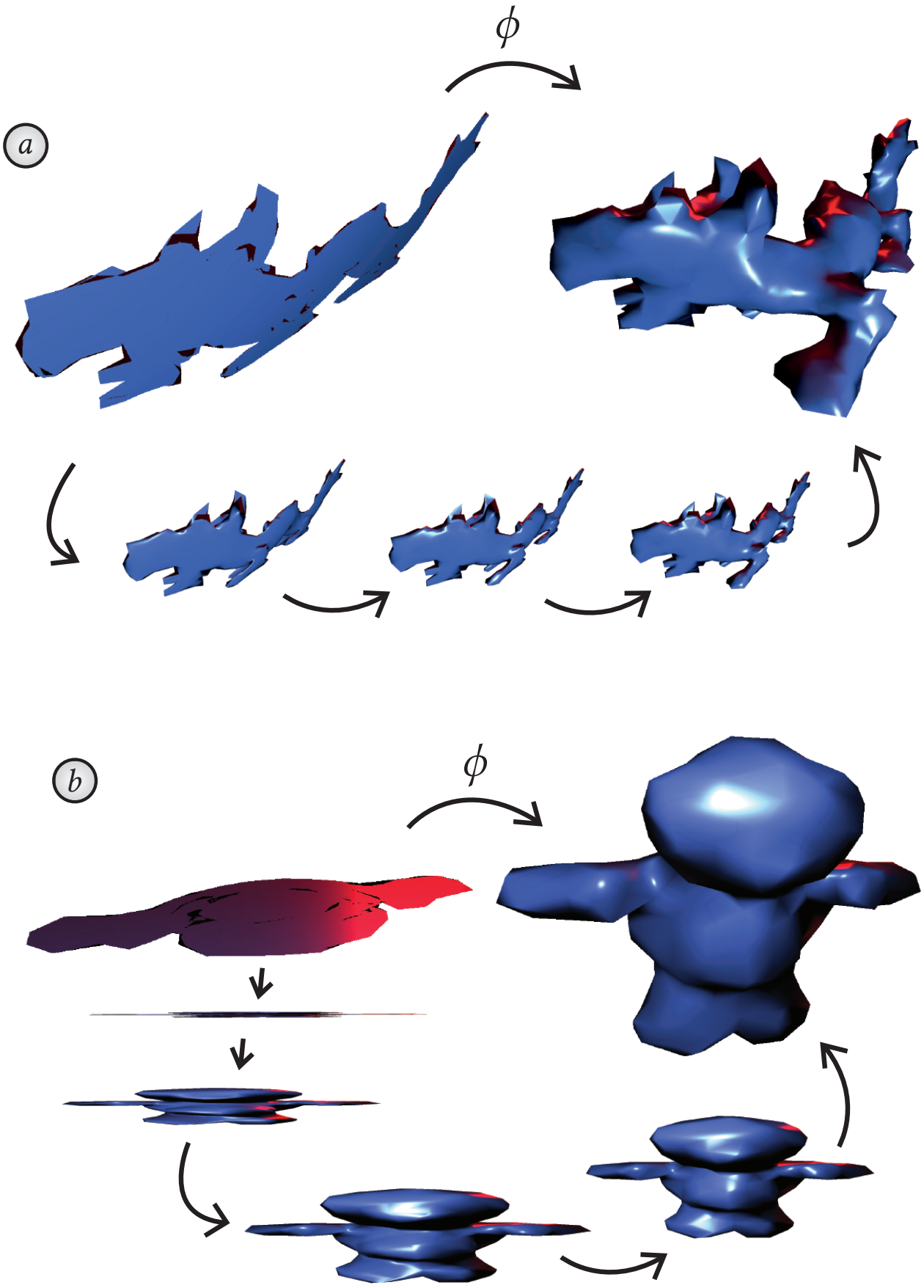


Figure 9.2: Results.

Chapter 10

Summary

In this thesis, after some brief introduction to the basics of computer graphics, FEM, and continuum mechanics, we looked at the craftsmanship of deformable simulators, mostly following the work of Smith et al. in [25] and [15]. Then, as an *'illustration'* of all the knowledge I've collected from the literature, I implemented a sample simulator in C++, then tested it out with some example models to arrive at a pretty sloppy summary you've read in the previous chapter.

I definitely had fun writing this thesis! All the work/research I've done brought not just FEM and continuum mechanics, but linear algebra and in general, math, much-much closer to me.
What's next? Here are the things I would like to do in the not so distant future:

1. The first thing I would like to do is to make the simulator *faster*. Probably you can already find an updated version at `marcisolti.github.io/ifem`.
2. After that it would be really nice to look into different *constitutive models*,
3. and what happens to them if I plug them into the *analytical eigendecomposition*.
4. The thing that also bugs me is the dynamic integration schemes' *stability*. What's up with that? I surely didn't spend enough time with experimenting, and I should try other schemes as well.

Appendices

Chapter A

An Introductory Example of FEM

Let's look at a nice example for FEM from [5]. Fig. A.1. shows a system of three rigid carts on a horizontal plane that are interconnected by a system of linear elastic springs. Calculate the displacements u_i of the carts for the f_i loading shown.

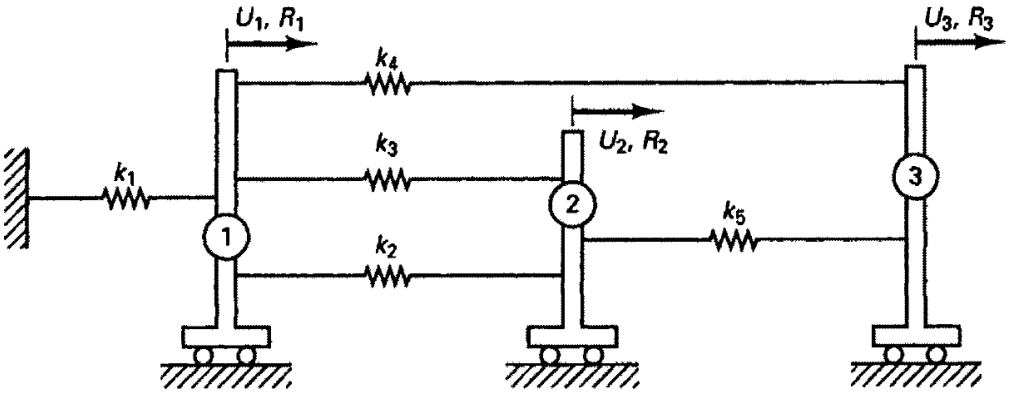


Figure A.1: Physical layout of the problem

A.1 System Idealization

We don't need to do much to *idealize this system.* The problem description already stated that the springs are *linear elastic* and the carts are *rigid.* The system is the assemblage of these idealized components – or *elements.*

A.2 Element Equilibrium

After *system idealization*, the next step is to establish the *equilibrium at each element i* in terms of the *state variables.* An *element* connects a number of points – called *nodes* – together in space. The *state variables* of a *node* is usually refers to its *spatial position* and the *forces acting on it.*

As the carts are in the horizontal plane, it is straightforward to assume that it can only move horizontally. Hence, our state variables are the u_is and the f_is, as shown on Fig. A.1. The *structural elements* will be the *linear elastic springs* connecting the carts.

A.2.1 Linear Elastic Spring as a Structural Element

The response of a linear elastic spring, that has one of its end attached to some fixed object, while the other end is pulled by some force of magnitude f, is calculated according to Hooke's law as

$$ku = f \tag{A.1}$$

Here the response is the displacement of the pulled end, denoted by u, while k is the *spring constant*. k is a positive, real number, complitely characterizing this ideal spring. See Fig. A.2 for reference.

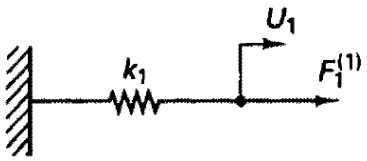


Figure A.2: A linear elastic spring with single degree of freedom

In this case, f can be thought of as some external *'energy'* which *'perturbates'* the system from its steady state. As a response, the system *'stores'* this energy in the spring itself, by equilibrating f with ku, hence the equation $ku = f$. In our problem, spring No. 1 is such a spring.

For the other springs in the system, both ends are free, so we have state variables u_1, u_2 and f_1, f_2. See Fig. A.3.

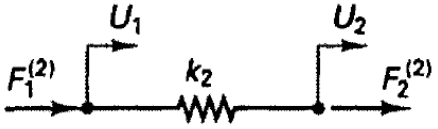


Figure A.3: A linear elastic spring with two degrees of freedom

The equilibrium now is a *system of equations*

$$\begin{aligned} k(u_1 - u_2) &= f_1 \\ k(-u_1 + u_2) &= f_2 \end{aligned} \tag{A.2}$$

which can be reformulated as

$$k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \tag{A.3}$$

We just defined the element equilibrium of a *1D linear elastic truss element*! In this equation,

$$k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} = \mathbf{K}^{(i)} \tag{A.4}$$

is the i^{th} element's *stiffness matrix*. Actually, Eq. A.3 and Eq. A.1 are the very same equation but with $u_1 = 0$ and $u_2 = u$. Nice!

Now we can go back to Fig. A.1 and define the element equilibrium for each element explicitly. The result can be seen on Fig. A.4.

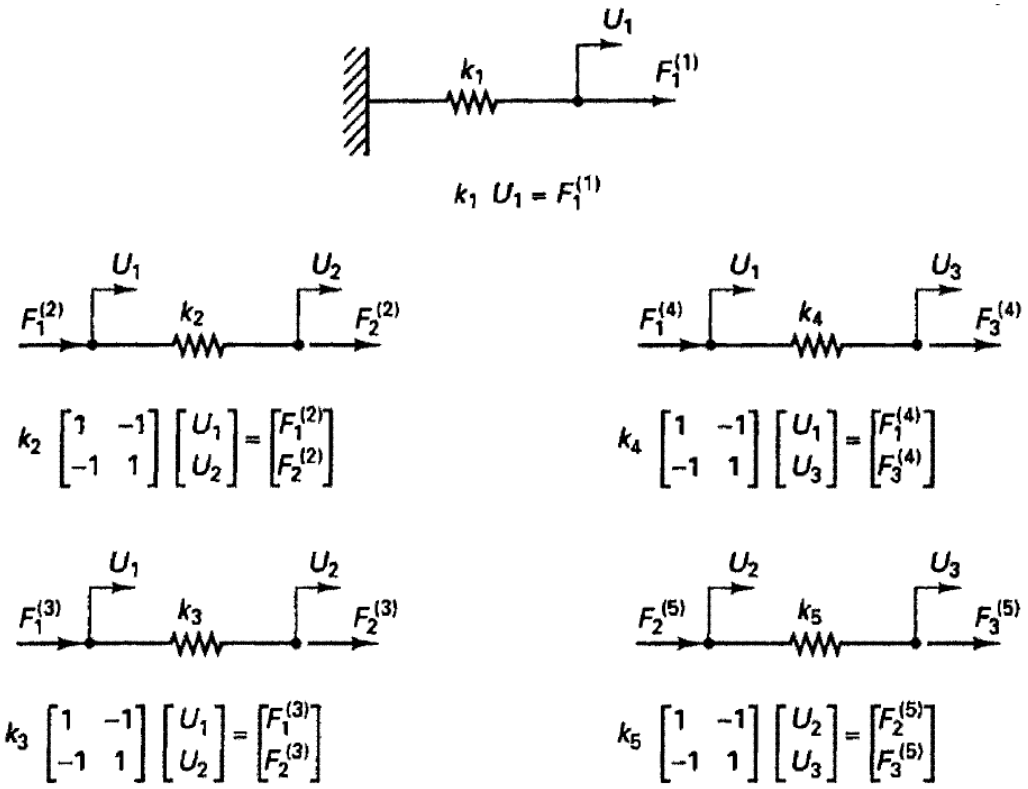


Figure A.4: Equilibrium at each element

A.3 Element Assemblage, Solution

To progress further, first we need to expand the element stiffness matrices to the global degrees of freedom. E.g. for the first element this means

$$\begin{bmatrix} k_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} f_1^{(1)} \\ 0 \\ 0 \end{bmatrix} \tag{A.5}$$

or

$$\mathbf{K}^{(1)}\mathbf{u} = \mathbf{f} \tag{A.6}$$

while for the second element

$$\begin{bmatrix} k_2 & -k_2 & 0 \\ -k_2 & k_2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} f_1^{(2)} \\ f_2^{(2)} \\ 0 \end{bmatrix} \tag{A.7}$$

or similarly

$$\mathbf{K}^{(2)}\mathbf{u} = \mathbf{f} \tag{A.8}$$

and so on.

To generate the governing equations for the state variables of the complete system, we need to invoke the element interconnection requirements. This will yield the *global stiffness matrix* **K**, which completely characterizes the *whole system's response.* In contrast, the *element stiffness matrices* characterized the *elements' response.*

The ultimate method for constructing the global stiffness matrix **K** is the *direct stiffness method*, but let's just not go down that road *yet.* Instead, consider the static equilibrium for each cart: $\sum f = 0$ According to the figure, this yields

$$\begin{aligned} f_1^{(1)} + f_1^{(2)} + f_1^{(3)} + f_1^{(4)} &= f_{\text{ext1}} \\ f_2^{(2)} + f_2^{(3)} + f_2^{(5)} &= f_{\text{ext2}} \\ f_3^{(4)} + f_3^{(5)} &= f_{\text{ext3}} \end{aligned} \tag{A.9}$$

In other words, the sum of all springs' (j) forces $f_i^{(j)}$ acting on each cart (i) are equal to the external forces $f_{\text{ext } i}$ introduced to the system.

We can now substitute the equilibriums of the element stiffness matrices in the interconnection requirements for the element end forces. With some symbolic machete slashing, this reduces to the fundamental equation of the Finite Element Method:

$$\boxed{\mathbf{Ku} = \mathbf{f}_{ext}} \tag{A.10}$$

where

$$\mathbf{K} = \begin{bmatrix} (k_1 + k_2 + k_3 + k_4) & -(k_2 + k_3) & -k_4 \\ -(k_2 + k_3) & (k_2 + k_3 + k_5) & k_5 \\ -k_4 & -k_5 & (k_4 + k_5) \end{bmatrix} \tag{A.11}$$

Here, **K** the global stiffness matrix, which completely characterizes the response of the system. Now you solve $\mathbf{Ku} = \mathbf{f}_{\text{ext}}$ for **u** to acquire the displacements in case of a specific loading condition $\mathbf{f}_{\text{ext}}$.

A.4 Other Lumped-Parameter Models

It has to be noted that the lumped-parameter mathematical model can be used in many other areas of physics.

Two classic examples of that are the steady-state pressure and flow distributions in the hydraulic network shown in Fig. A.4, and the steady-state current distributions in a DC network, as of Fig. A.4. In both cases, you can write the system of equation for each element for the currents entering and leaving the element at the ends, then use the very same assembly process to get the global system of equations.

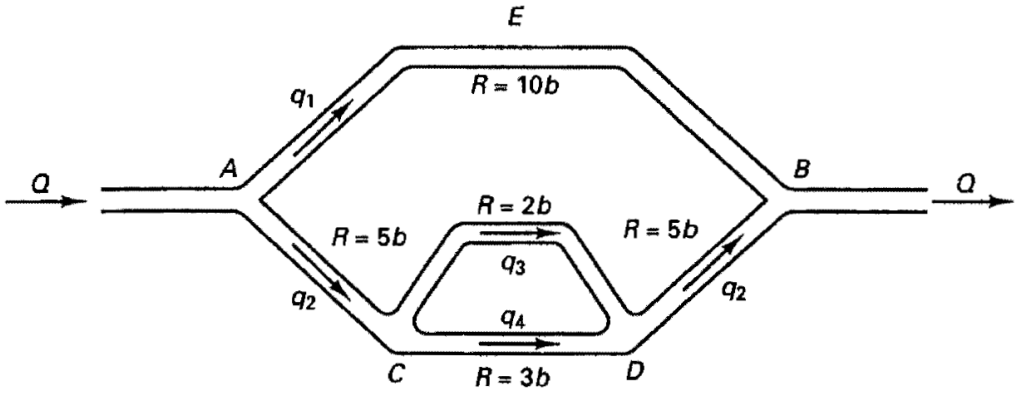


Figure A.5: Pipe network

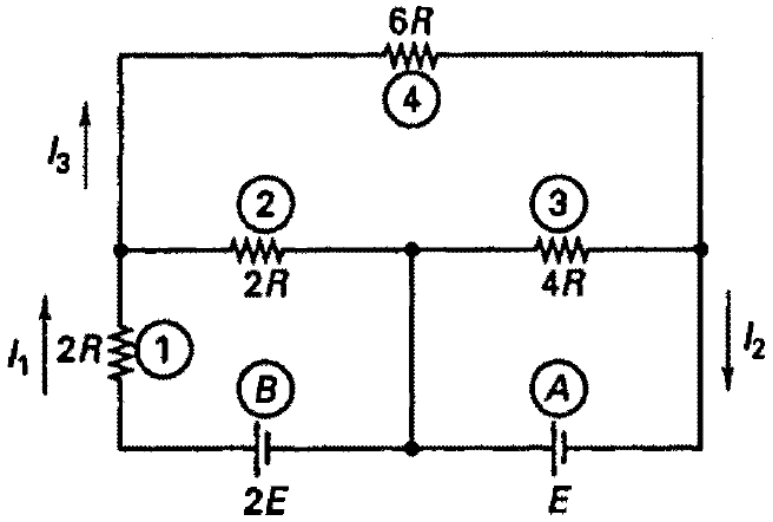


Figure A.6: DC network

Chapter B

The Method of Steepest Descent

B.1 What is a Linear System, Anyways?

Let's solve a linear system iteratively, following [23]. Consider the following linear system – illustrated on Fig B.1:

$$\mathbf{Ax} = \mathbf{b} \tag{B.1}$$

$$\mathbf{A} = \begin{bmatrix} 3 & 2 \\ 6 & 6 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} 2 \\ -8 \end{bmatrix} \tag{B.2}$$

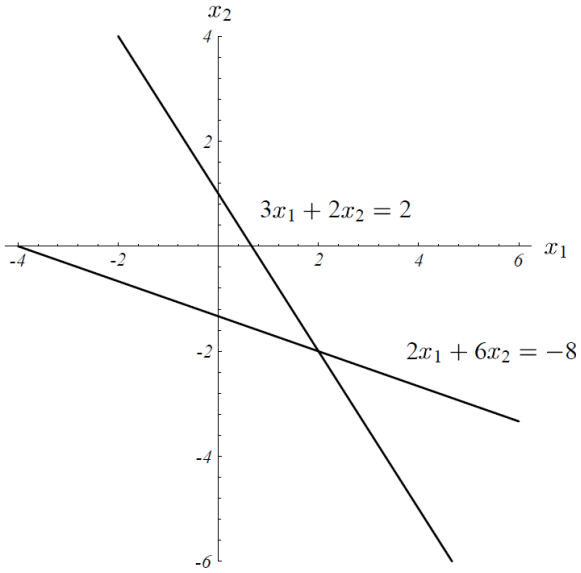


Figure B.1: Sample two-dimensional linear system. The solution lies at the intersection of the lines.

The *quadratic form* of such system is simply a scalar, quadratic function of a vector with the form

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{Ax} - \mathbf{b}^T\mathbf{x} + \mathbf{c} \tag{B.3}$$

where c is a scalar constant, $c = 0$ in our case. The graph and the contour plot of the *quadratic form* can be seen on Fig. B.2 – a picture is indeed worth a thousand words.

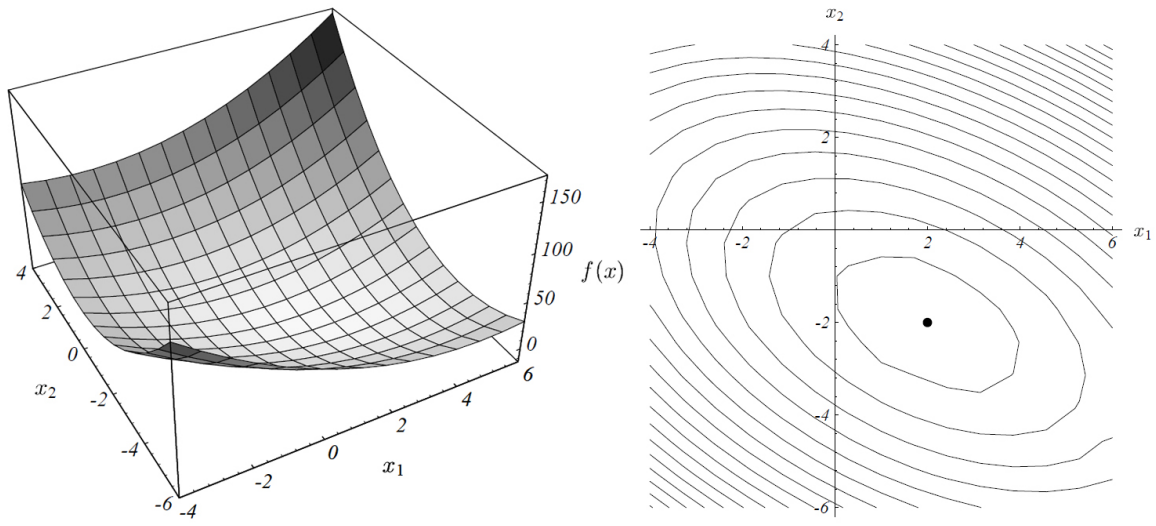


Figure B.2: a – Graph of a quadratic form $f(\mathbf{x})$. The minimum point of this surface is the solution to $\mathbf{Ax} = \mathbf{b}$. b – Contours of the quadratic form. Each ellipsoidal curve has constant $f(\mathbf{x})$

The *gradient* of a quadratic form is defined as

$$f'(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \frac{\partial}{\partial x_2} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_n} f(\mathbf{x}) \end{bmatrix} \tag{B.4}$$

This is visualized at Fig. B.3. With some tedious math, combining Eq. B.3 and B.4 yields

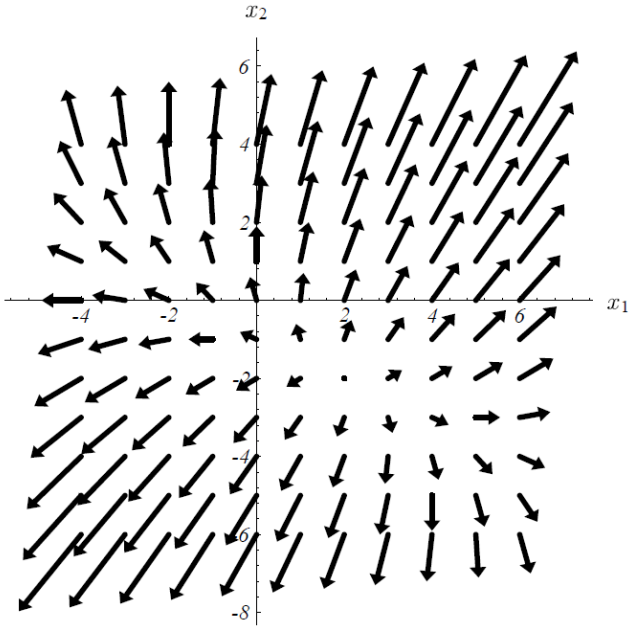


Figure B.3: Gradient $f'(\mathbf{x})$ of the quadratic form. For every x_i, the gradient points in the steepest increase of $f(\mathbf{x})$, and is orthogonal to the contour lines.

$$f'(\mathbf{x}) = \frac{1}{2}\mathbf{A}^T\mathbf{x} + \frac{1}{2}\mathbf{Ax} - \mathbf{b} \tag{B.5}$$

and if **A** is symmetric, this further reduces to

$$f(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b} \tag{B.6}$$

Setting the gradient to zero, we obtain the original linear system we want to solve. Isn't this wonderful? If **A** os positive-definite and symmetric, then solving $\mathbf{A}\mathbf{x} = \mathbf{b}$ for $\mathbf{x}$ equals minimizing $f(\mathbf{x})$. Other cases are illustrated on Fig. B.4

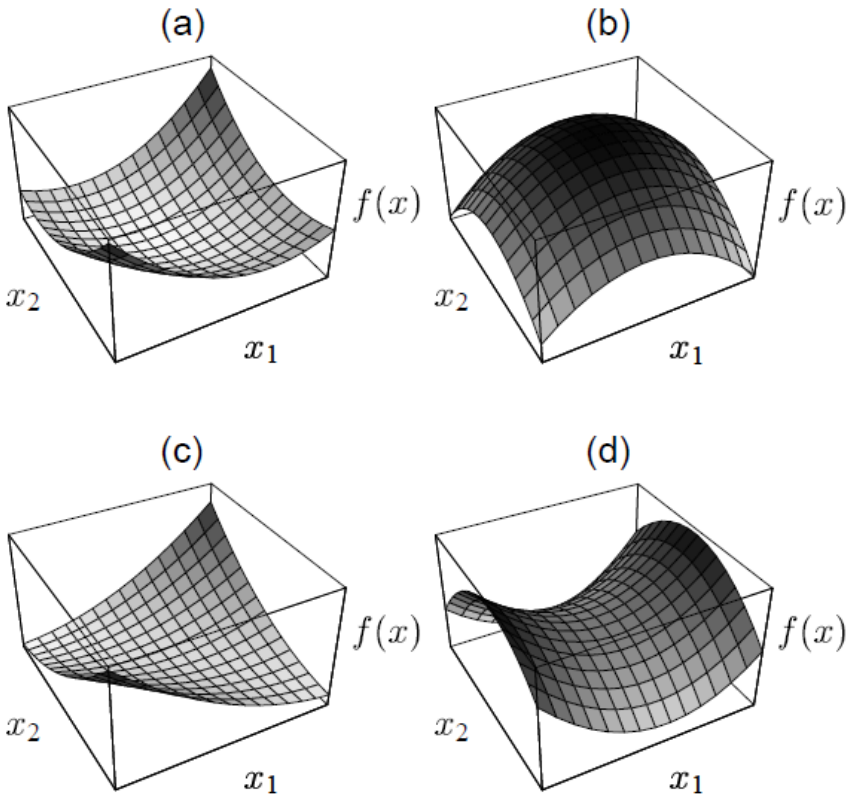


Figure B.4: a – quadratic form for a positive definite matrix. b – for a negative-definite matrix. c – for a singular (and positive-indefinite) matrix. A line that runs through the bottom of the valley is the set of solutions. d – For an indefinite matrix. Because the solution is a saddle point, Steepest Descent will not work. In three dimensions or higher, a singular matrix can also have a saddle.

In my opinion Fig. B.4 demonstrates pretty well why it is so important that **A** has to be positive- (or negative-) definite for an iterative method to work. You probably already have an intuition of what we are going to do next.

B.2 The Method of Steepest Descent

Next up: apply the method of Steepest Descent to solve the system of equations in discussion. As I stated in the introduction of the chapter, iterative method needs some intial value $\mathbf{x}^{(0)}$ as a starting point. We can choose this randomly for now, but in case of a real, n-dimensional problem, we would need to choose one near the equilibrium.

We now have this arbitrary starting point; in the method of Steepest Descent we'll slide down to the bottom of the paraboloid, by taking a series of steps $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$, ... until we are satisfied that we are close enough to the solution.

When we take a step, we choose the direction in which f decreases the quickest, which is the direction opposite $f'(\mathbf{x}^{(i)})$. According to Eq. B.6, this direction is $-f'(\mathbf{x}^{(i)}) = \mathbf{b} - \mathbf{A}\mathbf{x}^{(i)}$.

This direction is so important, that it has it's own name... and we've already heard about it! The residual $\mathbf{r}^{(i)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(i)}$ indicates how far we are from the correct value of $\mathbf{b}$; so whenever you read/hear *residual* think of it as the *direction of steepest descent*.

Suppose that we start at $\mathbf{x}^{(0)} = [-2, -2]^T$ Our first step, along the direction of steepest descent, will fall somewhere on the solid line in Fig. B.5a In other words, we will choose a point

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha \mathbf{r}^{(0)} \tag{B.7}$$

The question is, how big of a step should we take?

A line search is a procedure that chooses α to minimize α along a line. Fig. B.5b illustrates this task: we are restricted to choosing a point on the intersection of the vertical plane and the paraboloid. Fig. B.5c is the parabola defined by the intersection of these surfaces. What is the value of α at the base of the parabola?

Of course, we know from basic calculus that α minimizes f when its directional derivative is zero – see Fig. B.5d. Note that $r^{(0)}$ and $f'(\mathbf{x}^{(1)})$ are orthogonal.

The example is run until it converges in Fig. B.6. Not bad, however, note the zigzag path, which would appear because each gradient is orthogonal to the previous gradient. Wouldn't it be better if, every time we took a step, we got it right the first time? Sure it would and the method of conjugate gradients does that. If you've gotten excited, read the original paper: [23].

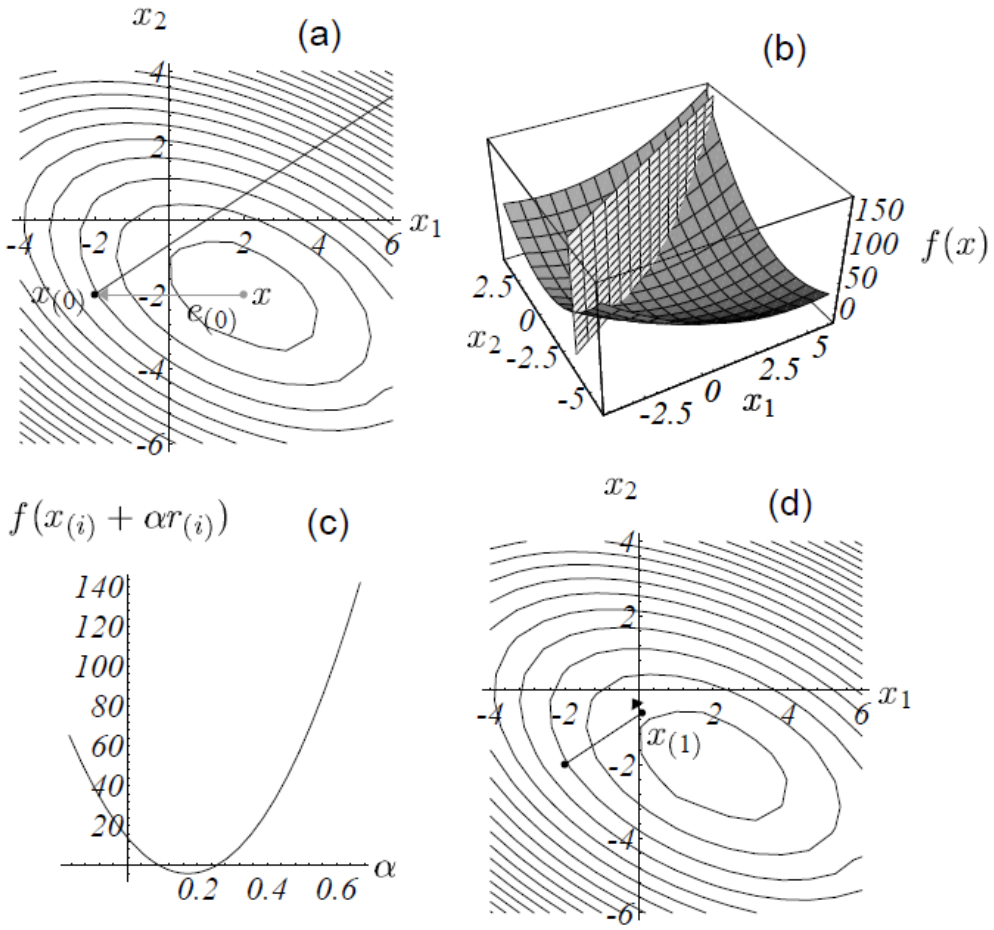


Figure B.5: The method of Steepest Descent. a – Starting at $[-2, -2]^T$, take a step in the direction of steepest descent of f. b – Find the point on the intersection of these two surfaces that minimizes f. c – This parabola is the intersection of surfaces. The bottommost point is our target. d – The gradient at the bottommost point is orthogonal to the gradient of the previous step.

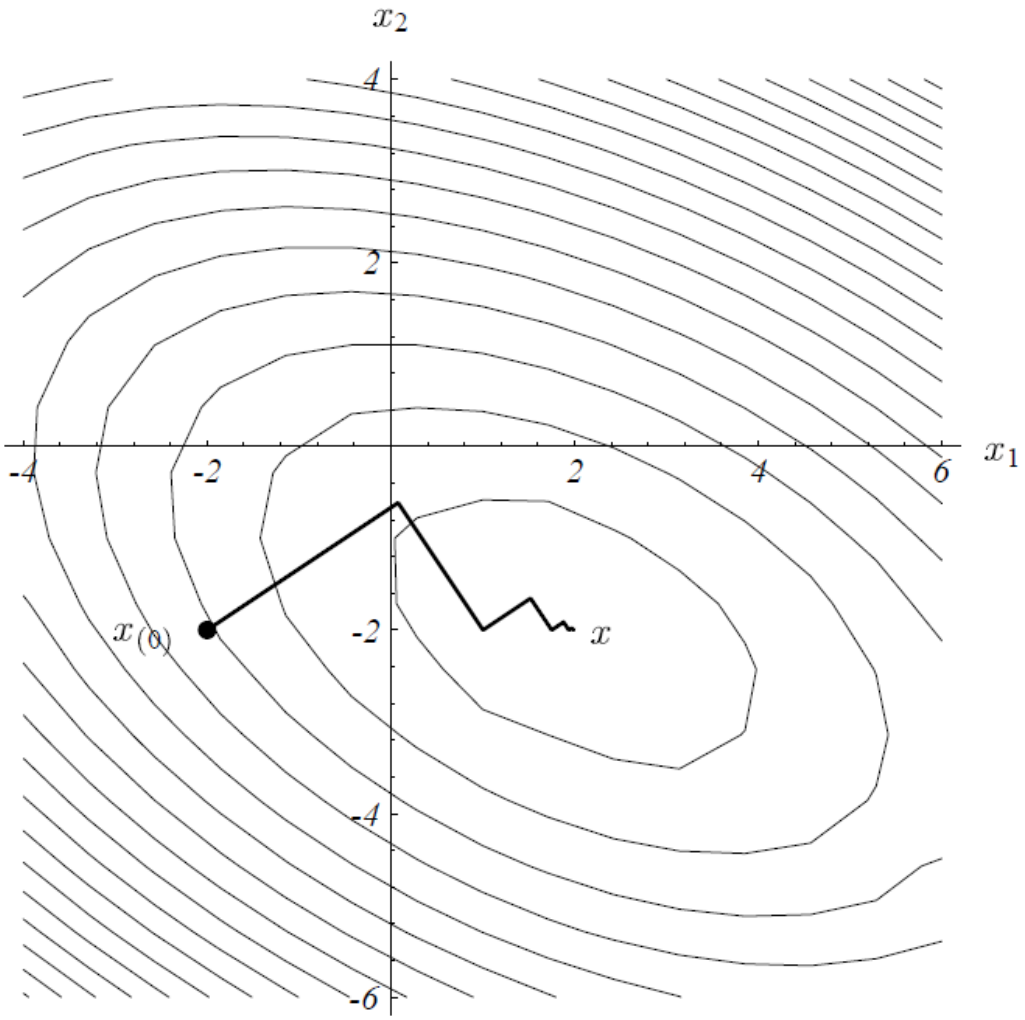


Figure B.6: The method of Steepest Descent starts at $[-2,-2]^T$ and converges at $[2,-2]^T$.

Chapter C

A Config File

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      "nu": 0.2,
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      "beta": 1.0
    },
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        "t": 0.0
      },
      {
        "f": 1000.0,
        "t": 1.0
      },
      ...
    ]
  }
}
```

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