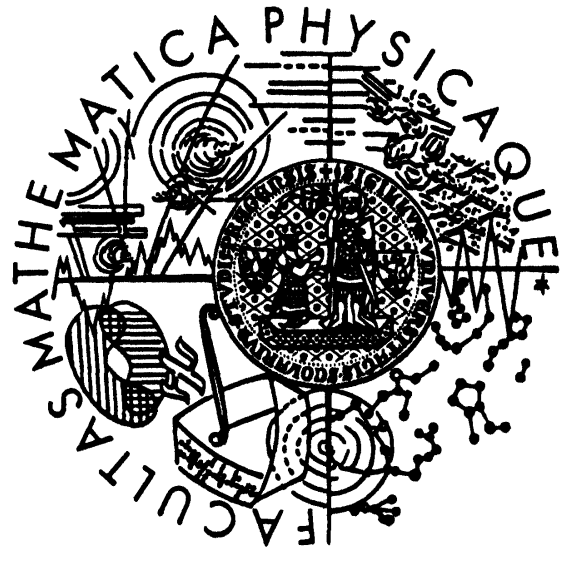
Charles University at Prague
Faculty of Mathematics and Physics

MASTER'S THESIS



Martin Mádlík

Viscous flow in elastic vessels
self-excited oscillation analysis

Mathematical Institute of Charles University
Supervisor: Prof. Ing. František Maršík DrSc.
Study branch: Mathematical modelling in physics and technics

I would like to thank all these people for help with this work. Without them it would not have been possible for me to finish it.

prof. Maršík My supervisor - neverending optimist

Dr. Hron Autor of (Hron, 2001), who helped me with program writing as much as he could

Dr. Knobloch Navier Stokes theoretical specialist

Ing. Buček Director of MikroVOX company - who lent me computers for computational experiments

My family For emotional support

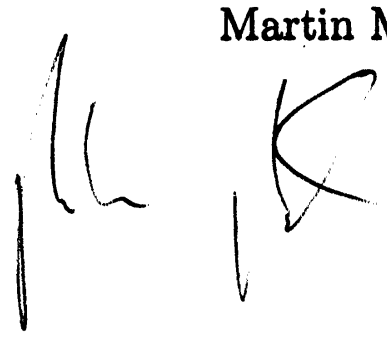
Ing. Špinka My friend, who helped me with my English

E. Kaspříková For help with my English and enormous support

Prohlašuji, že jsem svou diplomovou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce.

V Praze dne 16.4.2004

Martin Mádlík



CONTENTS

Název práce: Vazké proudění tepnou - analýza samobuzených oscilací
Autor: Martin Mádlík
Katedra (ústav): MUUK
Vedocí diplomové práce: Prof. Ing. František Maršík DrSc.
e-mail vedoucího: marsik@it.cas.cz

Abstrakt: Práce se zabývá odvozením a aplikací metody pro popis interakce proudového pole a elastické látky. Využívá přístupu mechaniky kontinua za použití ALE (Arbitrary Lagrange Euler) souřadnic a demonstruje celý přístup na problému tepenného proudění. Možnosti metody ukazuje při odvození dvou typů modelů. Pro vzniklý nestacionátní nelineární problém formuluje numerickou metodu a přikládá výsledky ve 3 prostorových dimenzích za použití vlastního programu pro řešení.
Klíčová slova: ALE, Fluid-Structure Interaction

Title: Viscous flow in elastic vessels - self oscillations analysis
Author: Martin Mádlík
Department: MUUK
Supervisor: Prof. Ing. František Maršík DrSc.
Supervisor's e-mail: marsik@it.cas.cz

Abstract: This work presents the derivation and application of a method for fluid structure interaction description. It employs the methods of continuum mechanics with usage of the ALE (Arbitrary Lagrange Euler) coordinates. It demonstrates the whole approach to problem of artery flow. The possibilities of this method are shown on the derivation of two models. The numerical method is formulated for the non stationary and nonlinear problem and some results are presented in three space dimensions, computed by a program, which was especially written for this purpose.
Keywords: ALE, Fluid-Structure Interaction

I would like to thank all these people for help with this work. Without them it would not have been possible for me to finish it.

prof. Maršík My supervisor - neverending optimist

Dr. Hron Autor of (Hron, 2001), who helped me with program writing as much as he could

Dr. Knobloch Navier Stokes theoretical specialist

Ing. Buček Director of MikroVOX company - who lent me computers for computational experiments

My family For emotional support

Ing. Špinka My friend, who helped me with my English

E. Kaspříková For help with my English and enormous support

Prohlašuji, že jsem svou diplomovou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce.

V Praze dne 16.4.2004 Martin Mádlík

NOTATION

Bold typeset means tensor, vectors are denoted by arrow

$\boldsymbol{C}$	Left Cauchy-Green stress tensor
c_v	specific heat
c_1, c_2	parameters for Mooney-Rivling material
dv, dv_y, dV	fundamental volume
$d\vec{a}, d\vec{A}$	fundamental surface
e_i	basis in $I\!R^N$
$\boldsymbol{I}$	Indentity
$\boldsymbol{F}$	deformation gradient
$\vec{\mathcal{F}}, \vec{f}$	external forces
k_n	time step
$\mathcal{L}$	Total quantity flux
m	Body mass
$\boldsymbol{M}$	internal production of angular momentum
$\vec{n}_\nu$	unit outer normal
p	pressure
$\mathcal{P}$	Total quantity production
$\boldsymbol{P}$	1st Piola-Kirchhoff stress tensor
$\underline{p}_k$	FE basis functions
q, Q	heat flux
$\widetilde{q}, \widetilde{Q}$	internal energy production
$\boldsymbol{R}$	Rotation part of deformation gradient
s, S	Entropy
t	time
T	Temperature
$\boldsymbol{t}$	Cauchy stress tensor
$\vec{u}$	displacement
$\boldsymbol{U}$	Displacement part of deformation gradient
$\underline{\vec{u}}_k$	FE basis functions
$\vec{v}$	velocity
$\underline{\vec{v}}_k$	FE basis functions
$\mathcal{V}_0$	Referential volume
$V_{(t)}$	Control volume
$\mathcal{V}_{(t)}$	Actual volume
W	Free Energy
$\vec{x}$	deformation
$\vec{X}$	material point in inital state

$\vec{y}$	arbitrary deformation
β	density paramater
Γ	domain boundary
ε	internal energy
η	test functions
θ	time integration parameter
λ	barycentrical coordinates
μ	viscosity
$\vec{\xi}$	test functions
Π	Dissipation energy
ϱ	Density
$\vec{\varsigma}$	test functions
Φ, φ	General quantity
Ψ	Helmholtz potential
Ω	Domain

INTRODUCTION

Mathematical modeling is a branch of mathematics dealing with the description and analysis of many processes around us. It tries to characterize these processes in other ways than experimental, and therefore is useful mainly in branches where experimental knowledge can be destructive. The application of this modeling approach in bio-engineering is one of many with very good results.

The urgency of studying the human cardiovascular system is quite apparent from the fact, that a great percentage of people of the western civilization die of cardiovascular diseases. A good model of blood flow in arteries could help physicians to reveal arteriosclerosis, warn patients of the possible risk of heart attack, or help with the treatment of collapsible brain arteries.

There are lot of problems connected with flow in the human body. They include many effects and interactions (mechanical, chemical, electrical). The journey to a model reasonably close to reality will probably be very long and difficult. In our work we will concentrate on the interaction of the velocity field with an elastic body, which seems to be the most essential in the description of artery flow.

There exist many different ways to characterize this problem. Some of them reduce the problem to the description of the artery wall, as in (Štembera, 2003). This problem is formulated as axially symmetric and the result is a one dimensional description of the deformation of the artery wall by the pulsating flowing fluid. The other models try to decompose the problem into two different parts: the flowing fluid and elastic deformation of the wall. Both parts are treated separately with well known and well tested methods, and the problem is solved by moving from one part to the other with each iteration. This approach sometimes has problems with the description of the interacting boundary. It is common in technical practice to combine two commercial programs together.

In our work, we will introduce a different approach. From the beginning the problem is formulated on a domain including the fluid and solid parts and is described by equations covering the deformation and velocity fields. This approach can be found e.g. in the work of (Hron, 2001). It is relatively difficult to derive this method because it has to overcome the differences between the description of the flowing fluid (usually using the Euler characterization) and the solid deformation (Lagrange description).

In our work we will derive the most general model of fluid-structure interaction, which we shall later simplify by adding two assumptions (well accepted in biology) of incompressibility and isotermicity. Unfortunately the

problem is too complicated for us to give any analytical properties, instead of that we will try to give some numerical results. We will try to catch many effects using 3D unstructured meshes.

ANATOMY

From the thermodynamic point of view, the human body is an open system. It consists of many small elements (cells) and it interacts with the environment (i.e. exchange of matter and energy between the body and the environment). It is an organism, which transforms the energy extracted from food to other forms, such as mechanical or mental work. The body consists of great amounts of cells (osteocytes, myocytes, ganglions, etc.), which must be nourished and the products of their metabolism must be drained. In the body of mammals this function is ensured by the cardiovascular system - a system of channels, which transports blood through out the whole body.

2.1 Cardiovascular system

The cardiovascular system (CVS) is a closed system of pipes, in which the blood flows. This system is powered by the heart, which is literally a pump, pumping the blood through the whole system. We may distinguish two types of pipes, or blood channels - arteries, which distribute the blood from the heart to the body, and veins, which convey the blood back from the body to the heart.

2.2 The heart

We have already pointed out that the heart is the driving organ of the whole CVS. Now let us describe its function in a more detailed way. The heart consists of three main parts: myocardium, which is the central layer, wrapped by endocardium and epicardium. The size of the heart depends on the weight and height of the person - it is approximately 280-340 g for men and 230-280 g for women. There are four hollows in the myocardium - left and right atrium and left and right ventricle. Respective atriums and ventricles are detached by aortic valves - there is the tricuspid valve between the right atrium and the right ventricle, and the mitral valve between the left ventricle and the left atrium. On the output of the right atrium there is the pulmonary semilunar valve, on the left atrium output there is the aortic semilunar valve. The heart is controlled by electrical impulses, which cause rhythmical contractions of the myocardium, where one contraction is one pulse. The amount of pulses per minute is called the heart frequency, which is normally 60-100 pulses per minute.

Over the course or the heart cycle two periods alternate:

Systole - a contraction of myocardium, which causes the blood to flow out of the heart

Diastole - a relaxation of myocardium, which causes the heart to fill with blood.

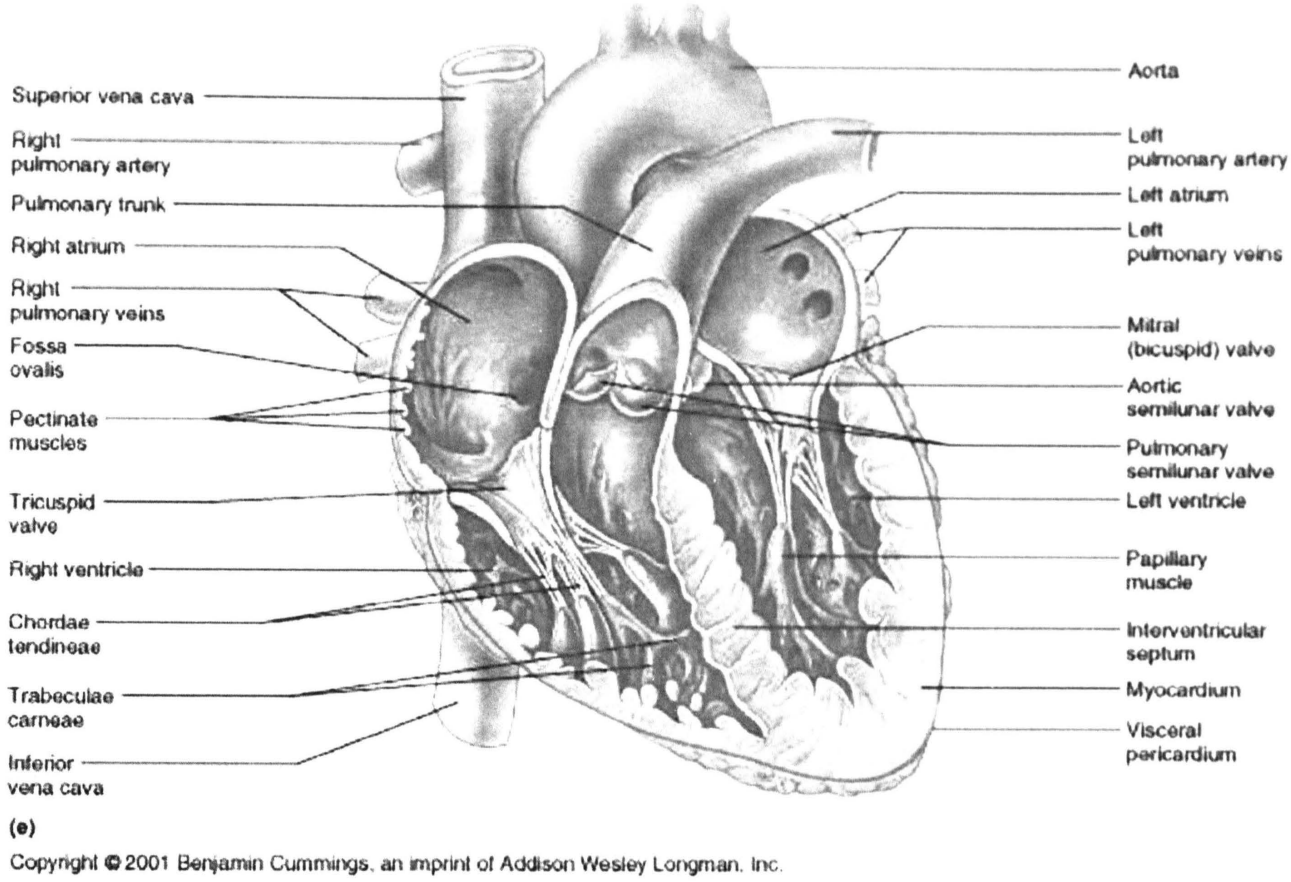


FIG. 2.2.1. The Heart

Table 2.2.1 *Systolic and diastolic pressure. Because of historical reasons the pressure is usually given in Torrs, 1 Torr = 133 Pa*

segment	systolic pressure [Torr]	diastolic pressure [Torr]
right atrium	8	2
right ventricle	15-30	0-8
pulmonary artery	10-30	5-15
left atrium	12	2
left ventricles	85 - 150	0 - 10
aorta	85-150	60-90

The heart cycle takes approximately 0.6-0.7 s, from which systole takes approximately 0.35 s and diastole 0.45 s. In normal circumstances the heart transfers approximately 5-7.5 l of blood per minute. The systolic and diastolic pressure are very important quantities used to describe the function of the heart, see the Table 2.2.1.

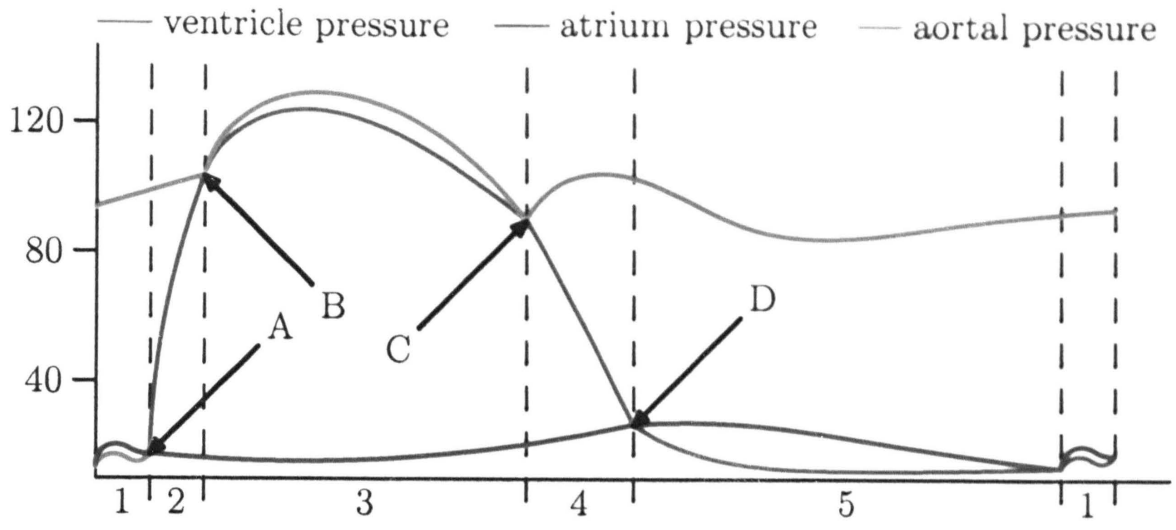
The heart cycle consists of five steps:

1. Systole of the atriums - A small amount of blood is forced to the ventricles, which were filled passively before.

2. Tensoidal systole of the ventricles - By that contraction the pressure in the ventricle increases, until the diastolic pressure in the artery is reached. The tricuspid and mitral valves are closing, while the output valves are opening. The blood is flowing from the heart into the body.

3. Systole of the ventricles - The volume of the ventricles reduces considerably and the output valves stay open.

4. Diastole of the ventricles - The pressure decreases rapidly and the volume changes. When the pressure reaches the diastolic level, the output



A - mitral valve closed, D mitral valve closed
B - aortal valve open, C aortal valve closed

FIG. 2.2.2. Heart cycle

valves close. The pressure in the ventricle decreases further until it reaches the pressure level at atriums, causing valves between the atriums and ventricles to open.

5. Passive filling - The blood is flowing into the heart spontaneously.

The complete course of the cycle is shown at Fig. 2.2.2.

2.3 The arteries

The blood is streaming from the heart by two arteries. One of them is the pulmonary artery leading from the right ventricle, and the other is aorta, leading from the left ventricle. The heart itself is supplied with blood by three coronary arteries, which detach directly from the aorta. The aorta is later slitted into the Common carotid, Left subclarion artery, Thoratic aorta and Aortic arch. The artery diameter is decreased by each division. This part of CVS is known as the high pressure part, for the blood is transported here by pressure strokes. The artery is conformable to this transport regime by its internal structure. At Fig. 2.3.3 we may see three layers, forming the artery wall. These layers are made of elastic material, which allows the actual volume of the artery to increase as the pressure stroke passes.

The arteries are further divided into arterioles. The parameters of the main arteries are noted in Table 2.2.1.

The coronary arterioles suppply oxygenated blood up to the individual cells, so it is obvious that they are very small. Therefore we no longer speak about flow, but rather about passive transport, for the arteriole is smaller in diameter than the transported molecule. We shall not consider this type of transport any further.

2.3.1 *Remodelation*

Every living tissue has the ability of persistent change and adaptation to the external conditions (the so-called remodelation). This property is partly enabled by the interaction (exchange of matter and energy) with environment. This interaction leads either to the preservation of the physiological

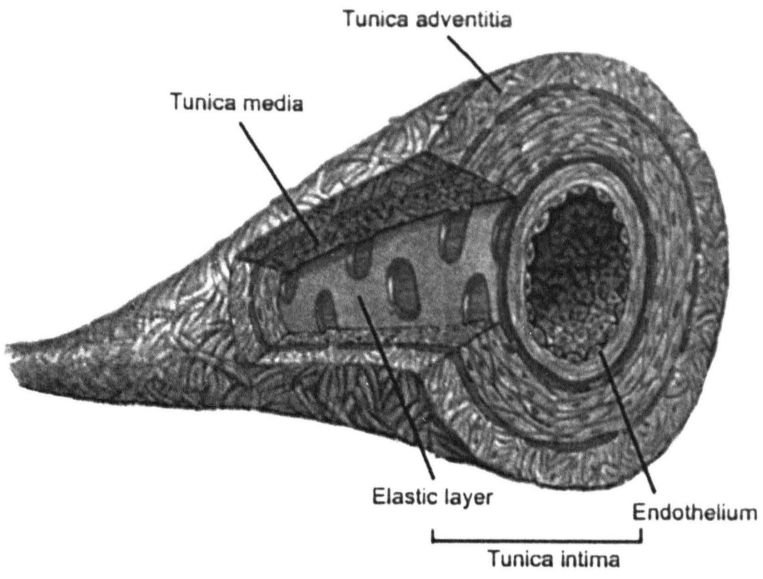


FIG. 2.3.3. Aorta

Table 2.3.2 *The list of arteries and their parameters*

artery	length [cm]	inner diameter [cm]	wall thickness [cm]
Ascending aorta	4	1.45	0.163
Common carotid	8.9	0.37	0.063
Internal carotid	11.8	0.15	0.042
Aortic arch	2.0	1.12	0.132
Left subclarion artery	3.4	0.42	0.067
Aortic arch	3.9	1.07	0.127
Thoratic aorta	5.2	1.0	0.120

properties or to their damage and malfunction. The examination of those properties is not possible without considering the dynamic effects of flowing blood. That is the reason for adding a model of mater exchange to the description of the artery wall in the next version of our model.

2.4 The veins

The blood with low oxygen volume and enriched by CO_2 is drained away from the cells by the venues, which later merge into veins. The master vein leads this blood into the right heart atrium. The structure of the vein is shown at Fig. 2.4.4. Because we are interested in the blood flow in the arteries, we shall not describe the veins any further.

2.5 The blood

Now let us briefly mention some basic facts concerning human blood, especially its composition and properties describing its characteristics as a fluid. Blood is a concoction of leukocytes, erythrocytes, thrombocytes and blood plasma, which consists mainly of proteins. The erythrocytes are elements with approximately $8\mu m$ in diameter and form the biggest part of blood in percentage terms (approx. 5.10^6 cells per 1 mm^3). These elements could be deformed due to shear stress. They represents approx. 95% of all blood elements. On the other hand there are much less leukocytes in human blood

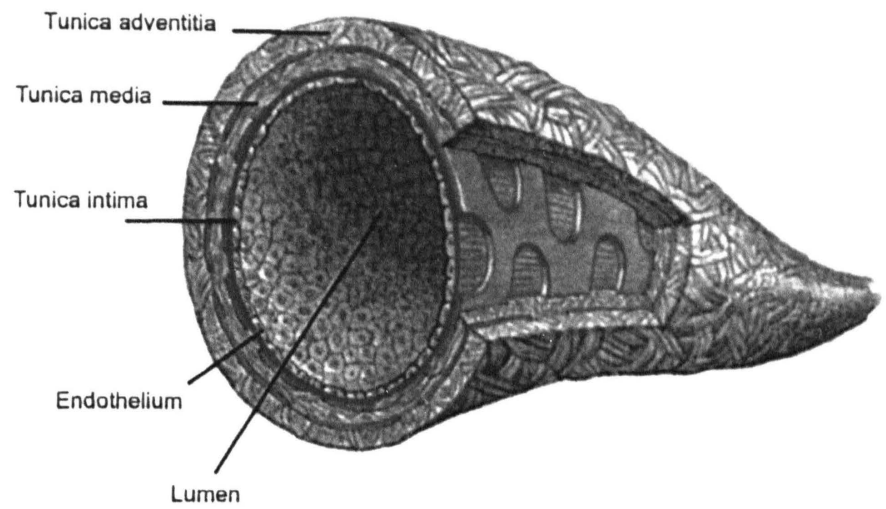


FIG. 2.4.4. Vein

- approx. 1 or 2 per 1000 erythrocytes. There are approx. 50-100 thrombocytes per 1000 erythrocytes, but their size is only 2 to 4 μm and at normal flow they can barely influence the blood properties.

The basic model describing the fluid from a mechanical point of view is the so-called Newton fluid. This theory assumes linear dependency of shear stress on shear velocity. It is expressed by the following formula (for brevity we use 1D approximation):

$$\tau = \eta \frac{dv}{dt} = \eta \dot{\gamma}.$$

The blood belogs to non-Newton fluids (that means the dependency of shear stress on shear velocity is non-linear, η in not a constant) and its rheological properties are still a subject of intensive research. It turns out that to describe all properties of blood as a whole is a rather complicated task. This is true because its properties vary significantly with shear velocity (see Fig. 2.5.5). It is shown there that for $\dot{\gamma} > 100$ blood behaves almost like a Newton fluid, but for $\dot{\gamma} \ll 100$ its behavior is significantly different. This is because at lower velocities its properties as a concoction are significant and different mechanical properties of respective elements begin to show. Let us mention the Casson's rheological model as an example of an empirical model, which approximates well the behavior of blood at lower speeds:

$$\tau = a^2 \dot{\gamma} + 2a\sqrt{\dot{\gamma} b} + b.$$

This model is more suitable for the description of flow in blood veins, other applications of this model are subject to debates ((J. Valenta *et al.*, 1995)). Because we shall consider the flow in big arteries, where big values of shear velocity are reached due to the pulse flow, we shall use the Newton model to describe the behavior of blood there.

2.6 Summary

In this chapter we have presented a rough insight into the anatomy of CVS, especially regarding the structure and function of the heart and the arteries. For computation purposes used in this work we have chosen the artery called

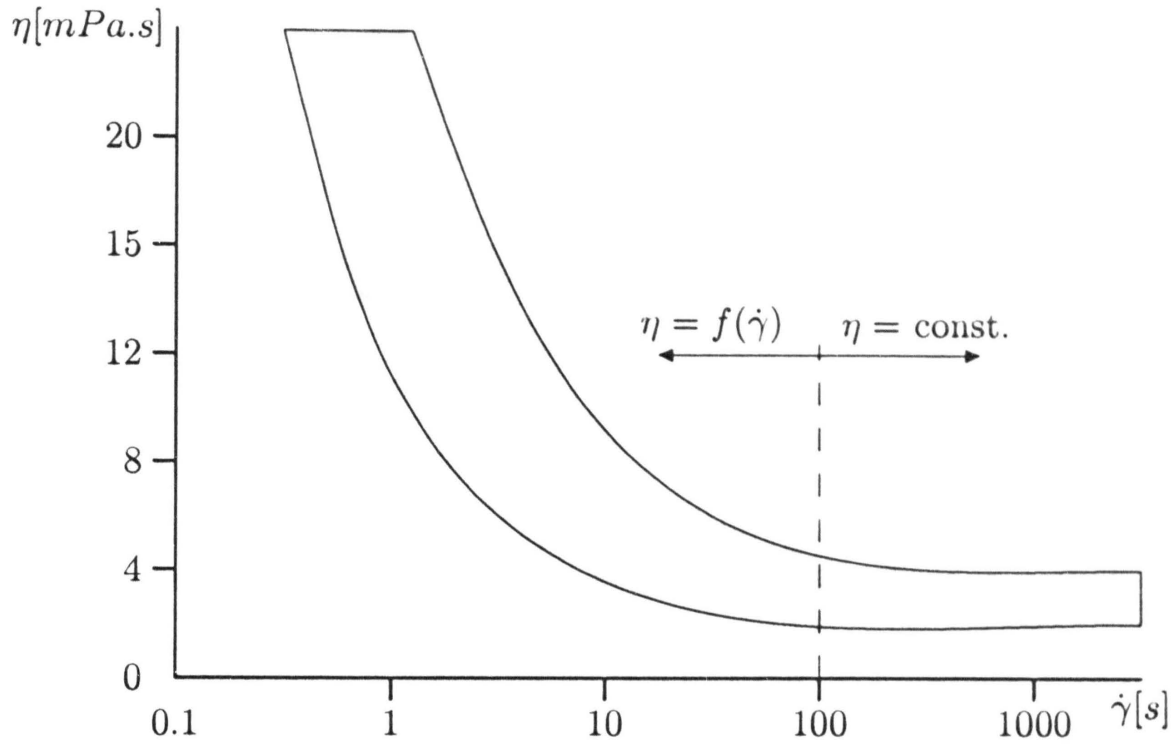


FIG. 2.5.5. Human blood viscosity η in dependence on shear velocity $\dot{\gamma}$.

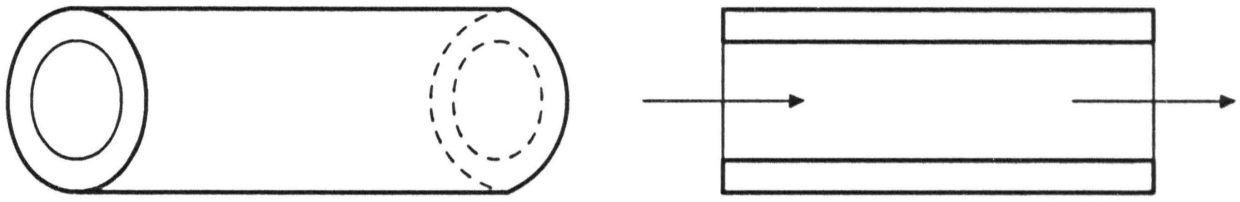


FIG. 2.6.6. Carotid in schematic view

carotid. In simplified form we may say we are interested in the flow of blood an in elastic pipe 89 mm long, with inner diameter 3.7 mm and wall thickness 0.63 mm, as shown at the Fig. 2.6.6.

The pipe changes its profile in dependence on the flow. The profile copies the pressure stroke caused by the contraction of myocardium.

PHYSICAL PROBLEM FORMULATION

In this chapter we will formulate a general model of fluid flowing in a solid tube. We will start in the most general manner, without any restrictive assumptions. Later we will use assumptions commonly used in biology, namely isothermalilty and incompressibility, and we will derive a simpler model, which will be used for numerical computations.

3.1 Continuum mechanics

First of all we have to find a way how to describe the fluid motion. Generally, there are two well-known principles of that description, called Lagrangian and Eulerian. But because our model requires a very special approach, we will set up another one, known as the ALE method.

3.1.1 *Motion description*

Imagine a body with volume $\mathcal{V}_0$ in some space. The body is free to move and to change its shape in time $t \in [0, T]$. Let us choose an arbitrary, but fixed configuration (which consists of the current position and shape of the body). We will call it *reference configuration* and we will express the motion and deformation of the body with respect to this configuration. Because the configuration of the body may change in time, we can describe the deformation process as a sequence of configurations.

More exactly : Let $\mathcal{V}_0 \in \mathbb{R}^3$ be the reference configuration of the body and $V_{(t)}$ an *actual configuration* (an arbitrary configuration in time t). The deformation is then defined as the mapping

$$\vec{x}_{\mathcal{V}} : \mathcal{V}_0 \times [0, T] \to \mathcal{V}_{(t)}.$$

The mapping $\vec{x}_{\mathcal{V}}$ depends on the choice of reference configuration. Let us assume that the reference configuration will always be the non-deformed

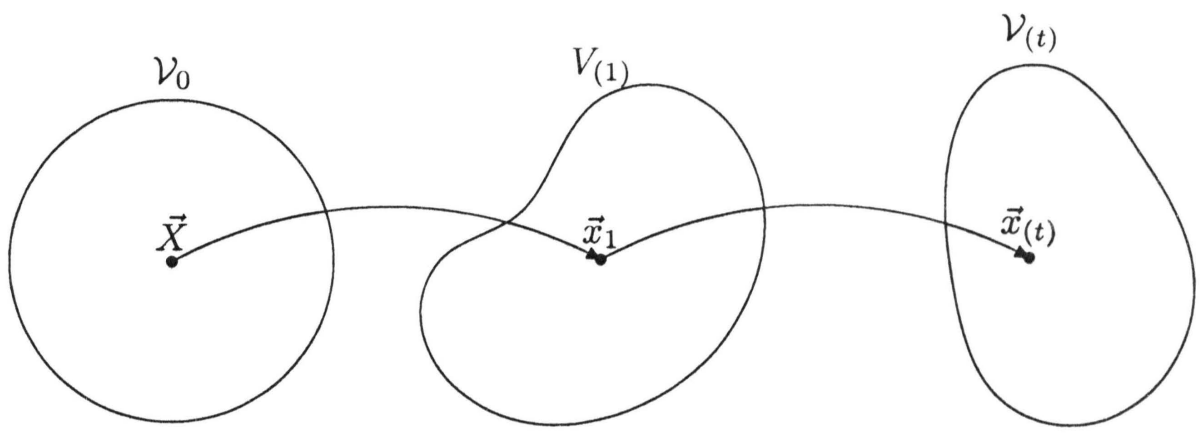


FIG. 3.1.1. Deformation from reference state $\vec{X}$ (volume $\mathcal{V}_0$) through intermediate state $\vec{x}_1$ (some volume $V_{(1)}$) to actual state $\vec{x}_{(t)}$ (actual volume $\mathcal{V}_{(t)}$).

state of the body denoted $\mathcal{V}_0$. In the words of formulas, we will assume that $\vec{x} = \vec{x}_{\mathcal{V}} = \vec{x}_{\mathcal{V}_0}$.

Reference positions of atomic elements of the body (also called *material points*) will be denoted $\vec{X}$. Their respective actual positions in the space are time-depend vectors denoted $\vec{x} = \vec{x}(\vec{X}, t)$.

Now, let us define the *displacement vector field* $\vec{u}$, which will be useful for the description of the properties of the deformed body

$$\vec{u}(\vec{X}, t) = \vec{x}(\vec{X}, t) - \vec{X}. \tag{3.1.1}$$

We shall also need the *velocity field*, defined as the time derivative of the position vector $\vec{x}$:

$$\vec{v} = \frac{\partial \vec{x}}{\partial t}. \tag{3.1.2}$$

The most important property of deformation is expressed by the *deformation gradient*

$$\boldsymbol{F} = \frac{\partial \vec{x}}{\partial \vec{X}} \text{ and its determinant } J = \det \boldsymbol{F}.$$

This newly defined quantity will be used to express the transformation between the reference and actual state. Let us mention the transformations of the fundamental surface and volume as an example:

$$dv = J\, d\mathcal{V} \qquad d\vec{a} = \boldsymbol{F}^{-T} J\, d\vec{A}.$$

3.1.1.1 *Lagrangian view* This approach is used to describe the motion of objects in some space. The main idea of this method can be explained as follows: choose an arbitrary point $\vec{X}$ on the body and trace its motion trough the space. The resulting trajectory is then given by the mapping $\vec{x} = \vec{x}(\vec{X}, t)$, where $\vec{X}$ denotes the initial position of the point in time $t = 0$. The coordinates $\vec{X}$ are also called *Lagrangian* or *material* coordinates.

The velocity of the material point is obviously given by the time derivative of its position:

$$\vec{v} = \dot{x} = \frac{\partial \vec{x}(\vec{X}, t)}{\partial t}. \tag{3.1.3}$$

With some additional assumptions (implicit function theorem) there also exists an inverse mapping

$$\vec{X} = \vec{X}(\vec{x}, t), \tag{3.1.4}$$

which allows us to derive $(\vec{X}, t)$ from $(\vec{x}, t)$.

Because the formulas 3.1.3 and 3.1.4 are inverse, it is obvious that

$$\frac{\partial x^i}{\partial X^I}\frac{\partial X^I}{\partial x^j} = \delta^i_j, \qquad \frac{\partial X^I}{\partial x^i}\frac{\partial x^i}{\partial X^J} = \delta^I_J,$$

where the tensor $\frac{\partial x^i}{\partial X^I}$ is the *deformation gradient*, denoted as $\boldsymbol{F} \equiv F^i_I$.

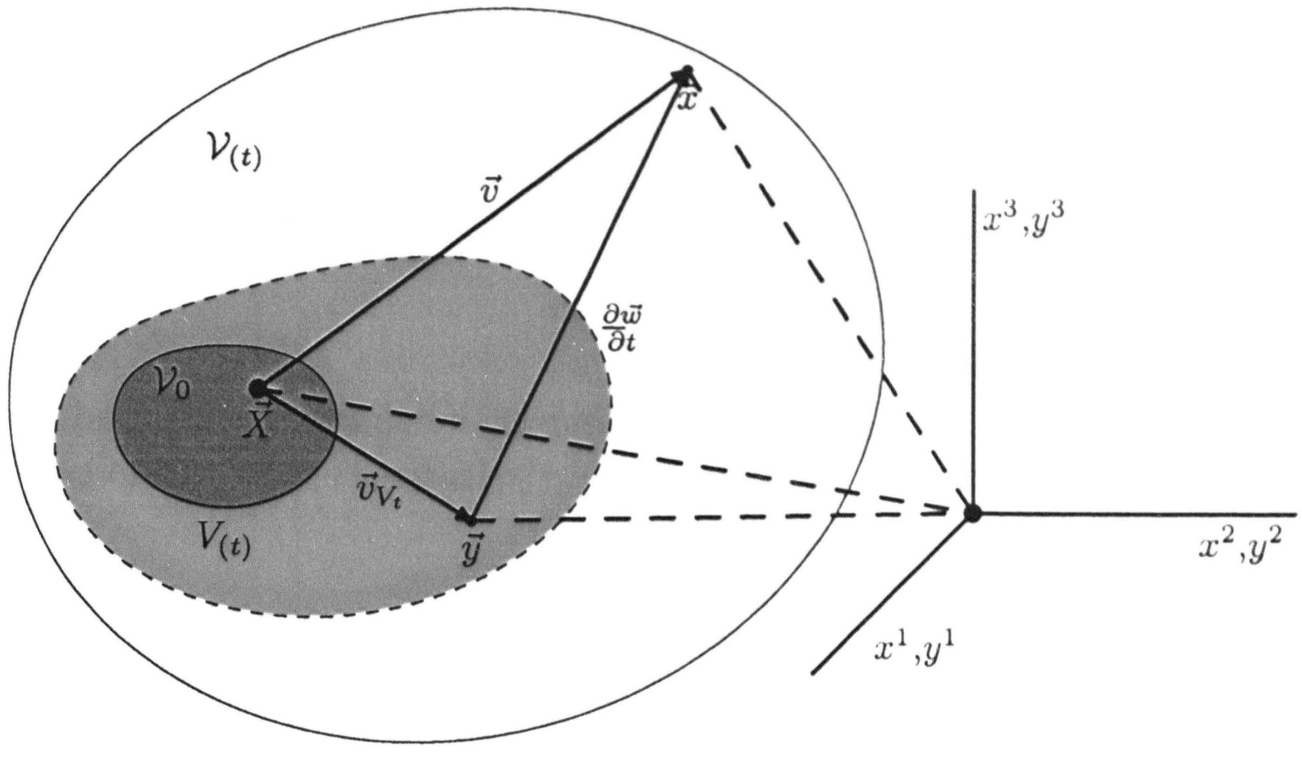


FIG. 3.1.2. ALE description; Material point $\vec{X}$ can be mapped to actual position $\vec{x}$ using arbitrary mapping $\vec{y}: \mathcal{V}_0 \times [0,T] \to V_{(t)}$ for description.

3.1.1.2 *Eulerian view* Euler's method is suitable for the description of a variable vector field in an invariant domain. It is based on the following idea: choose an arbitrary point $\vec{x}$ in the space and inspect all the elements passing through this point in time. The coordinates x^i are called *Euler* or *spatial* coordinates.

Velocity in the spatial coordinates can be expressed using 3.1.4 as

$$\vec{v} = \vec{v}(\vec{X},t) = \vec{v}(\vec{X}(\vec{x},t),t) = \vec{v}(\vec{x},t). \tag{3.1.5}$$

Analogically, we may transform any function $f(\vec{X},t)$ to $f(\vec{x},t)$ and vice versa, where $f(\vec{X},t)$ or $f(\vec{x},t)$ is a function describing any property of a material or spatial point, respectively.

The material derivation of the property function f in the spatial coordinates can be assessed from the derivation of a composite function

$$\dot{f}(\vec{x},t) = \frac{\partial f(\vec{x},t)}{\partial t} + v^i(\vec{x},t)\frac{\partial f(\vec{x},t)}{\partial \vec{x}^i}. \tag{3.1.6}$$

3.1.1.3 *ALE* The ALE (Arbitrary Lagrange Euler) method is a generalization of the previously described methods. It is similar to the Euler description, but the inspecting point $\vec{x}$ is not fixed anymore, and is free to move along an arbitrary vector $\vec{y}$ with velocity $\vec{v}_{V_t} = \frac{\partial \vec{y}}{\partial t}$.

It gives us the opportunity to establish the control volume $V_{(t)}$ which can be deformed by deformation $\vec{y}$. The deformation is expressed with respect to the y^i coordinate system.

Now look at Figure 3.1.2. The body $\mathcal{V}_0$ is in the reference configuration, which means it is in the non-deformed state. Let us deform the body in time t to the state $\mathcal{V}_{(t)}$ by the deformation $\vec{x} = \vec{x}(\vec{X},t)$. We will describe

this deformation using the coordinate system $[y^1, y^2, y^3]$ connected with deformation $\vec{y} = \vec{y}(\vec{X}, t)$ and deforming the control volume $V_{(t)}$. Now we have to express position

$$\vec{y}(\vec{X}, t) = \vec{x}(\vec{x}, t) - \vec{w}(\vec{X}, t) \tag{3.1.7}$$

and velocity

$$\frac{\partial \vec{y}}{\partial t} = \vec{v}_{V_t} = \vec{v} - \frac{\partial \vec{w}}{\partial t} \tag{3.1.8}$$

of the material point. Of course, such important property as the deformation gradient cannot be omitted:

$$\frac{\partial x^i}{\partial y^j} = \frac{\partial x^i}{\partial X^I} \frac{\partial X^I}{\partial y^j}. \tag{3.1.9}$$

Now we can try to express a material derivation of a function f in the y^i coordinate system. The idea is similar to the Euler description, but we shall use the velocity described by 3.1.8. The result is

$$\dot{f}(\vec{x}, t) = \frac{\partial f(\vec{x}, t)}{\partial t} + (v^i - v^i_{V_t})(\vec{x}, t) \frac{\partial f(\vec{x}, t)}{\partial \vec{x}^i}. \tag{3.1.10}$$

3.1.2 *Balance Laws*

To establish our model, we will also need equations describing the basic physical principles, known as the *balance laws*. Because our approach is a very general one, we will formulate them all in the ALE coordinates. The following concept will be used later for the description of fluid structure problems.

3.1.2.1 *General balance law in ALE coordinates* For derivation purposes, let us define a general extensive quantity $\Phi(t)$:

$$\Phi(t) = \int_{\mathcal{V}_0} \Phi(\vec{X}, t) d\mathcal{V} = \int_{\mathcal{V}_{(t)}} \varphi(\vec{x}, t) dv = \int_{V_{(t)}} \varphi(\vec{y}, t) dv_y.$$

The general balance law may be formulated in various ways. Let us choose the following one:

Time change of extensive quantity is compensated by the sum of total flux and total production.

If we denote the flux by $\mathcal{L}$ and the production by $\mathcal{P}$, we may write this law as follows:

$$\frac{d\Phi}{dt} = \dot{\Phi} = \mathcal{L}(\Phi) + \mathcal{P}(\Phi). \tag{3.1.11}$$

Our next goal is to quantify the flux and the production in the reference volume $\mathcal{V}_0$ in order to obtain a local balance. Let us start with flux:

$$\mathcal{L}(\Phi) = \int_{\partial \mathcal{V}_0} \mathcal{L}^K(\Phi) d\mathcal{A}_K = \int_{\partial \mathcal{V}_{(t)}} l^k(\Phi) da_k = \int_{\partial V_{(t)}} l^k(\Phi) \vec{n}_{k,V_t} da.$$

The total production is given by the density of production Σ, σ

$$\mathcal{P}(\Phi) = \int_{\mathcal{V}_0} \Sigma(\Phi) d\mathcal{V} = \int_{\mathcal{V}_{(t)}} \sigma(\Phi) dv = \int_{V_{(t)}} \sigma(\Phi) dv_y.$$

We may now compute the time change (time derivative) of Φ over the control volume $V_{(t)}$. This can be done using the 1st Reynolds transformation theorem:

$$\frac{d}{dt}\int_{V_{(t)}} \phi(\vec{y},t) dv_y = \frac{d}{dt}\int_{V_{(t)}} \phi(\vec{y},t) dv_y + \int_{\partial V_{(t)}} \phi(v^k - v^k_{V_t}) n_{k,V_t} da.$$

The boundary term on the right side of the previous equation means that flux is flowing on a non-material surface, which is our case, because the ALE control volume has nothing to do with the real boundary of the volume.

And finally we will transform the equations from control volume (which is changing in time) into the referential one (which is fixed in time) and put the derivation inside the integral.

Bearing in mind the transformation formula of the fundamental volume and surface, which is

$$dv_y = j_y d\mathcal{V} \ , \ n_{k,V_y} da = j_y \frac{\partial X^K}{\partial y^k} dA_K,$$

we will get

$$\frac{d}{dt}\int_{V_{(t)}} \phi(\vec{y},t) dv_y = \frac{\partial}{\partial t}\int_{\mathcal{V}_0} \phi(\vec{y}(\vec{X},t),t) j_y d\mathcal{V} = \int_{\mathcal{V}_0} \frac{\partial}{\partial t}\phi(\vec{y}(\vec{X},t),t) j_y d\mathcal{V}.$$

We may now apply the same procedure on the boundary term:

$$\int_{\partial V_{(t)}} \phi(\vec{y},t)(v^k - v^k_{V_t}) n_{k,V_t} da = \int_{\partial \mathcal{V}_0} \phi(\vec{y}(\vec{X},t),t)(v^k - v^k_{V_t}) j_y \frac{\partial X^K}{\partial y^k} dA_K.$$

After substituting these two terms into 3.1.11 we get the balance law in an integral form:

$$\int_{\mathcal{V}_0} \frac{\partial}{\partial t}\Phi j_y d\mathcal{V} + \int_{\partial \mathcal{V}_0} \Phi(v^k - v^k_{V_t}) j_y \frac{\partial X^K}{\partial y^k} dA_K =$$
$$\int_{\mathcal{V}_0} l^k(\Phi) j_y \frac{\partial X^K}{\partial y^k} dA_K + \int_{\mathcal{V}_0} \sigma(\Phi) j_y d\mathcal{V}.$$

Assuming continuity of the integrand we can use the Gauss theorem, and we will finally get the local form of the general balance law in the ALE coordinates:

$$\boxed{\frac{\partial}{\partial t}(j_y \Phi) + \frac{\partial}{\partial X^K}\left\{\left[\Phi(v^k - v^k_{V_t}) - l^k(\Phi)\right] j_y \frac{\partial X^K}{\partial y^k}\right\} - j_y \sigma(\Phi) = 0}. \tag{3.1.12}$$

3.1.2.2 *The balance of mass* We may formulate this law as follows: *The time change of mass is zero.* Imagine a body with volume $\mathcal{V}$ and total mass $m(t) = \int_{\mathcal{V}_0} \varrho(\vec{X}, t) d\mathcal{V} = \int_{\mathcal{V}_{(t)}} \varrho(\vec{x}, t) dv$. Therefore, if we substitute this mass m into general local balance formula 3.1.12, we shall get

$$\frac{\partial}{\partial t}(j_y \varrho) + \frac{\partial}{\partial X^K}\left\{\left[\varrho(v^k - v^k_{V_t})\right] j_y \frac{\partial X^K}{\partial y^k}\right\} = 0.$$

On the previous formula we can easily show that ALE is a generalization of the Lagrangian and Eulerian view. Let $V_{(t)}$ be the static control volume. This means that $\vec{y} = \vec{X}$, therefore $j_y = 1$ and $\frac{\partial X^K}{\partial y^k} = \delta^K_k$, $\frac{\partial}{\partial X^K} = \frac{\partial}{\partial x^l}\frac{\partial x^l}{\partial X^K}$. What remains is the Euler description:

$$\frac{\partial \varrho}{\partial t} + \frac{\partial(\varrho v^k)}{\partial x^k} = 0.$$

Now let $V_{(t)}$ be a flow, i.e. $(\vec{y} = \vec{x})$. This means that $j_y = j$, $\vec{v}_{V_{(t)}} = \vec{v}$ and $\frac{\partial X^K}{\partial x^k} = \overset{-1}{\boldsymbol{F}}{}^{\mathrm{K}}_{\mathrm{k}}$ is inverse to the gradient $\boldsymbol{F}^T$. We can now substitute and see the Lagrangian description:

$$\frac{\partial}{\partial t}(j\varrho) = 0.$$

3.1.2.3 *The balance of linear momentum* This balance expresses the equilibrium of all forces involved in the system. We may derive it by substituting the *total momentum* $\phi = \varrho v^i$ into the general balance law 3.1.12. The compensating terms represent surface forces, expressed by $l^k \sim t^{ki}$, where $\boldsymbol{t}$ is the Cauchy stress tensor. Forces are represented by the sources of $\vec{f}$, in the words of production $\sigma = \rho f^i$. After substitution we have

$$\frac{\partial}{\partial t}(j_y \varrho v^i) + \frac{\partial}{\partial X^K}\left\{\left[\varrho v^i(v^k - v^k_{V_t}) - t^{ki}\right] j_y \frac{\partial X^K}{\partial y^k}\right\} - j_y \varrho f^i = 0. \quad (3.1.13)$$

The Lagrangian view can be derived in a way similar to the one we have shown in 3.1.2.2. We use the Piola-Kirchhoff pseudo-stress tensor $\boldsymbol{P} = T^i = T^{Ki} N_K$ to describe the action of surface forces. It is required to depend only on the reference configuration in order to meet the demands of constitutive relations. We may write it as follows $T^{KI} = \frac{\partial X^I}{\partial x^i} T^{Ki}$. The tensor $\boldsymbol{T}$ is called the second Piola-Kirchhoff tensor.

The Lagrangian description takes the form

$$\varrho\left(\dot{\vec{v}}^i - \mathcal{F}^i\right) - \frac{\partial \boldsymbol{T}^{Ki}}{\partial X^K} = 0. \quad (3.1.14)$$

3.1.2.4 *The balance of angular momentum* The angular momentum is expressed as the external product of the vector $\overrightarrow{x - y_0}$ and momentum vector $\varrho\vec{v}$ in 3.1.12 $\phi = [\vec{x} - \vec{y}_0] \wedge \varrho\vec{v}$. We may split the sources of angular momentum into two separate parts: into external volume forces $[(\vec{x} - \vec{y}_0) \wedge \varrho f]^{ij}$ and all

the other volume forces acting on dipoles, expressed by ϱM^{ij}. Generalised fluxes have the form $[(\vec{x}-\vec{y}_0)\wedge t^{ij}]$. One of the possible ways to describe the local balance is

$$0=\frac{\partial}{\partial t}\left(j_y[(\vec{x}-\vec{y}_0)\wedge\varrho\vec{v}]^{ij}\right)-j_y\varrho M^{ij}-j_y[(\vec{x}-\vec{y}_0)\wedge\varrho f]^{ij}$$
$$-\frac{\partial}{\partial X^K}\left\{\left[[(\vec{x}-\vec{y}_0)\wedge\varrho\vec{v}]^{ij}(v^k-v^k_{V_t})-(\vec{x}-\vec{y}_0)\wedge t^k\right]^{ij}j_y\frac{\partial X^K}{\partial y^k}\right\}.$$

We can now simplify this formula by multiplying 3.1.13 by the position vector $(\vec{x}-\vec{y}_0)$

$$0=\frac{\partial}{\partial t}(j_y\varrho v^i)\wedge(\vec{x}-\vec{y}_0)+\frac{\partial}{\partial X^K}\left\{\left[\varrho v^i(v^k-v^k_{V_t})-t^{ki}\right]j_y\frac{\partial X^K}{\partial y^k}\right\}\wedge(\vec{x}-\vec{y}_0)$$
$$-j_y\varrho f^i\wedge(\vec{x}-\vec{y}_0).$$

After subtraction and evaluation of the derivation of external product we get

$$-j_y\varrho M^{ij}-\frac{\partial}{\partial X^K}\left\{\left[[(\vec{x}-\vec{y}_0)\wedge\varrho\vec{v}]^{ij}(v^k-v^k_{V_t})-(\vec{x}-\vec{y}_0)\wedge t^k\right]^{ij}j_y\frac{\partial X^K}{\partial y^k}\right\}$$
$$+\frac{\partial}{\partial X^K}\left\{\left[\varrho v^i(v^k-v^k_{V_t})-t^{ki}\right]j_y\frac{\partial X^K}{\partial y^k}\right\}\wedge(\vec{x}-\vec{y}_0)=0.$$

and if we transform this into spatial coordinates, we shall get

$$t^{ji}-t^{ij}=\varrho M^{ij}. \tag{3.1.15}$$

For non-polar materials (with $M^{ij}\equiv 0$) 3.1.15 expresses the symmetry of the stress tensor.

3.1.2.5 *The balance of mechanical of energy* The total amount of mechanical energy can be written as $\phi=\varrho\left(\frac{v^2}{2}\right)$. We can formulate it without flow through the boundary ($l^k\equiv 0$). Energy production is denoted by $\sigma=v_i\frac{\partial t^{ji}}{\partial x^j}+\varrho v_i f^i$. Then the local balance is

$$\frac{\partial}{\partial t}\left(j_y\varrho\left(\frac{v^2}{2}\right)\right)+\frac{\partial}{\partial X^K}\left\{\left[\varrho\left(\frac{v^2}{2}\right)(v^k-v^k_{V_t})\right]j_y\frac{\partial X^K}{\partial y^k}\right\}$$
$$-j_y\left(v_i\frac{\partial t^{ji}}{\partial x^j}+\varrho v_i f^i\right)=0.$$

3.1.2.6 *The balance of internal energy* Let ε be the internal energy per unit mass. This energy can flow through the boundary due to heat fluxes ($l^k=q^k$) and can be produced internally by $\sigma=t^{ji}\frac{\partial v_l}{\partial x^l}+\widetilde{q}$, where $\widetilde{q}$ can be some other internal production e.g. radiation.

The local balance is

$$\frac{\partial}{\partial t}(j_y\varrho\varepsilon)+\frac{\partial}{\partial X^K}\left\{\left[\varrho\varepsilon(v^k-v^k_{V_t})-q^k\right]j_y\frac{\partial X^K}{\partial y^k}\right\}-j_y\left(t^{kl}\frac{\partial v_k}{\partial x^l}+\widetilde{q}\right)=0. \tag{3.1.16}$$

3.1.2.7 *The balance of entropy* This balance is a representation of the 2nd Thermodynamic law. It will be useful for "validating" the constitutive relations. It is not an equality, but an inequality. Let s be the entropy per unit mass. Total fluxes are $l^k = -\frac{q^k}{T}$, where T is temperature. Entropy production is nonnegative and can be determined by $\sigma = \varrho\dot{s} + \frac{\partial}{\partial x^k}\left(\frac{q^k}{T}\right) - \frac{\tilde{q}}{T} \geq 0$.

The local balance follows simply from 3.1.12

$$0 \leq \frac{\partial}{\partial t}(j_y \varrho s) + \frac{\partial}{\partial X^K}\left\{\left[\varrho s(v^k - v^k_{V_t}) + \frac{q^k}{T}\right] j_y \frac{\partial X^K}{\partial y^k}\right\} - j_y\left(\varrho\dot{s} + \frac{\partial}{\partial x^k}\left(\frac{q^k}{T}\right) - \frac{\widetilde{q}}{T}\right).$$

3.1.2.8 *Density of dissipation energy* Energy dissipation is used more often then the balance entropy production as a representation of 2nd Thermodynamic law. It can be derived from entropy balance by eliminating heat fluxes and substituting internal energy balance.

First of all we need to express $\Sigma(S)$ and for that we need to transform flux from and into ref. configuration:

$$q^k = j_y^{-1}\frac{\partial y^k}{\partial X^K}Q^k, \qquad Q^k = j_y\frac{\partial X^K}{\partial y^k}q^k.$$

Now we can eliminate heat fluxes. We rewrite internal energy balance 3.1.16 with transformed fluxes:

$$\frac{\partial}{\partial t}\left(j_y \rho\varepsilon\right) + \frac{\partial}{\partial X^K}\left\{\rho\varepsilon\left(v^k - v^k_{V_t}\right) j_y \frac{\partial X^K}{\partial y^k}\right\} + \frac{\partial}{\partial X^K}Q^K - j_y t^{kl}\frac{\partial v_l}{\partial x^k} - \tilde{Q} = 0.$$

Now we can write the entropy production in reference configuration:

$$\begin{aligned}\Sigma(S) &= \rho\dot{s} + Q^K\frac{\partial}{\partial X^K}\left(\frac{1}{T}\right) + \frac{1}{T}\frac{\partial}{\partial X^K}Q^K - \frac{\tilde{Q}}{T} \geq 0\\ &= \rho j_y\dot{s} + Q^K\frac{\partial}{\partial X^K}\left(\frac{1}{T}\right)\\ &+ \frac{1}{T}\left(-\frac{\partial}{\partial t}\left(j_y\rho\varepsilon\right) - \frac{\partial}{\partial X^K}\left\{\left[\rho\varepsilon\left(v^k - v^k_{V_t}\right)\right] j_y\frac{\partial X^K}{\partial y^k}\right\} + j_y t^{kl}\frac{\partial v_l}{\partial x^k}\right) \geq 0.\end{aligned}$$

Density of dissipation energy is defined by $\Pi = T\Sigma(S)$:

$$\begin{aligned}0 \leq \Pi = T\Sigma(S) = &\\ &T\rho j_y\dot{s} + TQ^K\frac{\partial}{\partial X^K}\left(\frac{1}{T}\right) - \frac{\partial}{\partial t}\left(j_y\rho\varepsilon\right)\\ &- \frac{\partial}{\partial X^K}\left\{\left[\rho\varepsilon\left(v^k - v^k_{V_t}\right)\right] j_y\frac{\partial X^K}{\partial y^k}\right\} + j_y t^{kl}\frac{\partial v_l}{\partial x^k}.\end{aligned}$$

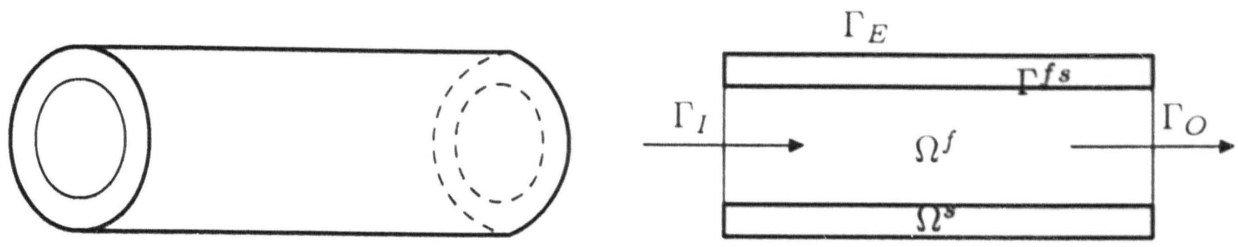


FIG. 3.2.3. Domain notation

3.2 General model of material system

Now we can formulate equations describing the solid deformation and the fluid motion. The idea of Fluid Structure Interaction in this model is very clear. The deformation of solid material will be described by the Lagrange method and the motion generated by deformation will be 'the arbitrary' motion of control volume in the ALE coordinates used for fluid motion description.

Remark 3.1. *Concerning notation Now we are going to describe the motion and deformation in the solid and fluid parts of our body. Let* Ω *be the body - you can imagine a vessel filled with blood (see 3.2.3). For brevity we use the upper index* ^{s} *behind a letter to describe the solid part and* ^{f} *for the fluid part and we use lower index* $_t$ *behind a letter to desribe actual configuration. We cannot forget to notate the boundary :* Γ^{fs} *is the boundary connecting the fluid and solid parts,* Γ_I *means input,* Γ_O *output and the remaining part will be noted as* Γ_E*.*

3.2.1 *Motion and deformation*

This will be the basis of our model. The deformation of the solid part will be described by the mapping $\vec{x}^s$

$$\vec{x}^s : \Omega^s \times [0,T] \to \Omega^s_t.$$

We calculate the displacement vector $\vec{u}^s$, which will be unknown in our model, from the relation

$$\vec{u}^s(\vec{X},t) = \vec{x}^s(\vec{X},t) - \vec{X}.$$

The velocity vector $\vec{v}^s$ is the time change of the position vector

$$\vec{v}^s(\vec{X},t) = \frac{\partial \vec{x}^s(\vec{X},t)}{\partial t}.$$

The main unknown in the fluid part will be the velocity field $\vec{v}^f$ defined in Ω^f

$$\vec{v}^f(\vec{x},t) : \Omega^f \times [0,T] \to \mathbb{R}^3.$$

For the description of change of domain Ω^f we introduce the mapping $\vec{y}$

$$\vec{y} : \Omega^f \times [0,T] \to \Omega^f_t,$$

which will be useful for defining the displacement vector $\vec{u}^f$ in Ω^f

$$\vec{u}^f(\vec{X},t) = \vec{y}(\vec{X},t) - \vec{X}. \tag{3.2.17}$$

The first paragraph in Chapter 3.2 reveals the main idea of our model. A part of this paragraph can be precisely formulated by prescribing properties for the virtual mapping $\vec{y}$

$$\vec{y}(\vec{X},t) = \vec{x}(\vec{X},t) \qquad \forall(\vec{X},t) \in \Gamma^{fs} \times [0,T]. \tag{3.2.18}$$

The second consequence of that paragraph concerns the velocity. Our model aims to describe the viscous flow interacting with the solid material. Remember what does the viscous assumption mean for the velocity boundary condition. Sometimes it is called "no slip", it prescribes zero velocity on solid boundary. Next, imagine that we are moving the solid boundary with displacement $\vec{u}^s$ and with velocity $\vec{v}^s$. It is clear, that we have to "copy" this motion in fluid, which directly leads to the interacting version of the non-slip boundary condition

$$\vec{v}^f = \vec{v}^s \qquad \text{on } \Gamma_t^{fs}.$$

When we denote $\Omega = \Omega^s \cup \Omega^f$ we can define new fields

$$\vec{u} : \Omega \times [0,T] \to \mathbb{R}^3,$$
$$\vec{v} : \Omega \times [0,T] \to \mathbb{R}^3,$$

by the following prescription

$$\vec{v} = \begin{cases} \vec{v}^s & \text{in } \Omega^s \\ \vec{v}^f & \text{in } \Omega^f \end{cases}$$
$$\vec{u} = \begin{cases} \vec{u}^s & \text{in } \Omega^s \\ \vec{u}^f & \text{in } \Omega^f. \end{cases}$$

The consequence of the relations 3.2.17 and 3.2.18 is the continuity across the boundary Γ_t^{fs}.

But the unification in not over yet. We can continue by introducing only one deformation gradient $\boldsymbol{F}$ and its determinant j

$$\boldsymbol{F} = \boldsymbol{I} + \nabla\vec{u}, \tag{3.2.19}$$
$$j = \det \boldsymbol{F}. \tag{3.2.20}$$

Now we can start formulating the equations describing the behavior of unknown functions. Unknowns in this model are (besides $\vec{u}$,$\vec{v}$): density ρ^s,ρ^f, temperature T^s, T^f, dissipative energy Π^s, Π^f, internal energy ε^s and ε^f.

Equations describing the solid part will be in Lagrange form, so the balance law can be simplified as previously shown on the example with mass balance

$$\frac{d}{dt}(\rho^s j) = 0. \tag{3.2.21}$$

The linear momentum balance follows

$$\rho^s j(\dot{v}^i - F^i) - \frac{\partial T^{Ki}}{\partial X^K} = 0. \tag{3.2.22}$$

Balance of internal energy

$$\rho^s \left(\frac{v^2}{2} + \varepsilon^s\right) - \frac{\partial}{\partial X^K}\left(T^{Ki} v_i - Q^K\right) - \left(\rho^s j F^i v_i + \tilde{Q}\right) = 0. \tag{3.2.23}$$

And the remaining balance is the dissipative energy balance

$$T^s \rho^s \left(T^s \dot{s}^s - \varepsilon^s\right) - \frac{Q^K}{T^s}\frac{\partial T^s}{\partial X^K} + T^{Ki}\frac{\partial v_i}{\partial X^K} \geq 0. \tag{3.2.24}$$

The equation describing grid deformation is also very important. In the solid part it is a natural definition of velocity

$$\frac{\partial u^i}{\partial t} = v^i. \tag{3.2.25}$$

A more complicated situation arises in the fluid part. We have already said that we use the ALE coordinates here. Now we must state what will be "the arbitrary" position vector exactly. We know, that it must correspond to the deformation of the solid part, therefore we use time derivative of displacement $\vec{u}$. Into the balance law we will put a substitution using 3.2.25. This mapping transforms the equations into referential configuration, which is the only one in which it is possible to write computable formulas.

In this way the balance of mass can be expressed as

$$\frac{\partial}{\partial t}\left(\rho^f j\right) + \frac{\partial}{\partial X^K}\left\{\left[\rho^f\left(v_k - \frac{\partial u^k}{\partial t}\right)\right] j\frac{\partial X^K}{\partial x^k}\right\} = 0. \tag{3.2.26}$$

The balance of linear momentum will be

$$\frac{\partial}{\partial t}\left(\rho^f v^i\right) + \frac{\partial}{\partial X^K}\left\{\left[\rho^f v^i\left(v^k - \frac{\partial u^k}{\partial t}\right) - t^{ki}\right] j\frac{\partial X^K}{\partial x^k}\right\} - j\rho^f f^i = 0. \tag{3.2.27}$$

The balance of internal energy is formally more complicated

$$\begin{aligned} 0 = & \frac{\partial}{\partial t}\left(j\varrho^f\left(\frac{v^2}{2} + \varepsilon^f\right)\right) - j\left(\varrho^f v_i + \tilde{q}\right) \\ & + \frac{\partial}{\partial X^K}\left\{\left[\varrho^f\left(\frac{v^2}{2} + \varepsilon^f\right)\left(v^k - \frac{\partial \vec{u}}{\partial t}\right) - t^{ki} v_i + q^k\right] j\frac{\partial X^K}{\partial x^k}\right\}. \end{aligned}$$

The most complicated formula in the whole work is the dissipative energy in fluid, if you don't believe it, continue reading

$$
\begin{aligned}
0 \quad \leq \quad & T^f \frac{\partial}{\partial t}\left(j\rho^f s^f\right) + T\frac{\partial}{\partial X^K}\left\{\varrho^f s^f\left(v^k - \frac{\partial u^k}{\partial t}\right) j\frac{\partial X^K}{\partial x^k}\right\} \\
& -\frac{\partial}{\partial t}\left(j\varrho^f \varepsilon^f\right) - \frac{\partial}{\partial X^K}\left\{\varrho^f \varepsilon^f\left(v^k - \frac{\partial \vec{u}}{\partial t}\right) j - \frac{\partial X^K}{\partial x^k}\right\} \\
& T^f Q^K \frac{\partial}{\partial X^K}\left(\frac{1}{T}\right) + jt^{ki}\frac{\partial v_i}{\partial x^k}.
\end{aligned}
$$

The remaining equation is the grid deformation. Here we can prescribe any equation, which can be easily solved, because there is no physical principle behind this. We choose the Laplace equation

$$
\frac{\partial u^k}{\partial t} = \frac{\partial^2 u^k}{\partial X^J \partial X^J}. \tag{3.2.28}
$$

As you can easily calculate we have 12 unknown functions and only 10 equations. It still remains to prescribe the terms $\boldsymbol{t}$ and $\boldsymbol{P}$. This is all done by closing equations and constitutive relations. We deal with it in the next chapter.

Remark 3.2 (About pressure). *You might have noticed there is no pressure in the list of unknowns. But this quantity is the only one which is important for technicians or doctors. Pressure p^s and p^f comes into the model through constitutive relations (e.g. Cauchy stress tensor $\boldsymbol{t} = \boldsymbol{t}(p, \dots)$). For more detailed description, refer to Chapter3.3.*

3.2.2 *Closing equations*

For our purposes, there should be two types of closing equations. The first one is not closing but simplification and will be stated by the assumption that the internal energy is constant. The second one is a group of closing relations called the state equations.

3.2.2.1 *State equations* This kind of equations is used for the description of fluids or solids where they change their phase. The formulas are derived from statistical physics and they are based on detailed study of the microscopical structure of material. We will not talk about derivation, instead we recommend to the reader to read (Maršík, 1999). For completeness we introduce

$$
p\left(T,\rho\right) = -3K\alpha\left(T - T_0\right) + K\left(\frac{\rho}{\rho_0} - 1\right) \tag{3.2.29}
$$

$$
p\left(T,\rho\right) = -\left(\frac{\rho}{M}\right)^2 a + \frac{\rho\hat{R}T}{M\left[1 - \frac{\rho}{M}b\right]} \tag{3.2.30}
$$

$$
p\left(T,\rho\right) = \frac{\rho\hat{R}T}{M} = \rho RT. \tag{3.2.31}
$$

These equations describe three phases : 3.2.29 solid materials (like steel), 3.2.30 is *van der Waals equation*, which can be used for the description of fluids even in phase changes and 3.2.31 gases with temperatures high above the condensing temperature.

3.2.2.2 *Internal energy* The remaining closing equation will concern internal energy. This simply means the assumption: the internal energy depends only on temperature T,

$$\varepsilon^s = c_v^s \left(T^s - T_0\right) + \varepsilon^s \tag{3.2.32}$$

$$\varepsilon^f = c_v^f \left(T^f - T_0\right) + \varepsilon^f, \tag{3.2.33}$$

where $c_v = \left(\frac{\partial u}{\partial T}\right)_\varrho$ is specific heat.

3.3 Constitutive relations

3.3.1 *Fluid Constitutive Relations*

In our work the constitutive relations mean the specification of $\boldsymbol{t}^f$. This formula will characterize the internal properties of fluid - dependence on pressure, velocity, etc. For testing purposes there is a very well known model of fluid - the Newtonian one

$$\boldsymbol{t}^f = -p^f \boldsymbol{I} + \mu \left(\nabla \vec{v}^f + \nabla^T \vec{v}^f - \frac{1}{3} \mathrm{div}\left(v^f\right) \boldsymbol{I} \right), \tag{3.3.34}$$

which assumes linear dependence, as we have discussed in the previous chapter.

3.3.2 *Constitutive Relations for Elastic Material*

The characteristics of solid material is described by the First Piola-Kirchhoff pseudo-stress tensor $\boldsymbol{P}$, as we have already mentioned. In this general part we only list some kinds of formulas, which are commonly used, but later in paragraph 3.5 we will introduce full derivation under some additional assumptions.

The prescription of $\boldsymbol{P}^s$ is

$$\boldsymbol{P}^s = -j p^s \boldsymbol{F}^{-T} + j \varrho^s \frac{\partial \Psi}{\partial \boldsymbol{F}}, \tag{3.3.35}$$

where Ψ is the Helmholtz potential. It can be shown, that Ψ depends only on the Left Cauchy-Green stress tensor $\boldsymbol{C}$ $(= \boldsymbol{F}^T \boldsymbol{F})$ and with this tensor we can describe the real reaction of material. The dependence can be written as $\Psi = \hat{\Psi}(\boldsymbol{C})$. We list two commonly used materials (neo-Hookean 3.3.36 and Mooney-Rivlin 3.3.37)

$$\hat{\Psi} = \frac{c_1}{\beta} \left(j^{-2\beta} - 1\right) + c_1 \left(I_C - 3\right), \tag{3.3.36}$$

$$\hat{\Psi} = c_1 \left(I_c - 3\right) + c_2 \left(II_C - 3\right) - d \ln j + c \left(j - 1\right)^2, \tag{3.3.37}$$

where I_C and II_C are the first and second invariants of $\boldsymbol{C}$ and d, β, c_1, c_2 are parameters. For more information about this topic see (Maršík, 1999) or (Humphrey, 2002).

3.4 Simple model

It is obvious, that the general model is too complicated for any practical use. Now we start with our simplification. There are two assumptions in biology, which are not far from reality: isotermicity, incompressibility.

3.4.1 *Consequences of assumptions*

These assumptions simply mean ϱ = const. and T = const. The simplification will be reflected in the equations and also in the constitutive relations. Some of the equations can even be omitted.

3.4.2 *Model formulation*

Now we take the equations from the general model one by one and apply our assumptions to them.

The balance of mass also known as the continuity equation is

$$0 = j - 1, \tag{3.4.38}$$

$$0 = \frac{\partial}{\partial X^K}\left(j v^k \frac{\partial X^K}{\partial x^k}\right). \tag{3.4.39}$$

The balance of linear momentum reduces to

$$\frac{dv^i}{dt} = \frac{1}{j\varrho^s}\frac{\partial \boldsymbol{T}^{Ki}}{\partial X^K}, \tag{3.4.40}$$

$$\frac{\partial v^i}{\partial t} = \frac{\partial}{\partial X^K}\left\{\left[v^i(v^k - \frac{\partial u^k}{\partial t}) - \boldsymbol{t}^{ki}\right]\frac{\partial X^K}{\partial x^k}\right\}. \tag{3.4.41}$$

The grid deformation equation follows

$$\frac{\partial u^i}{\partial t} = v^i, \tag{3.4.42}$$

$$\frac{\partial u^i}{\partial t} = \frac{\partial^2 u^i}{\partial X^J \partial X^J}. \tag{3.4.43}$$

The unknowns $\vec{v}$, $\vec{u}$ and p must fulfil the boundary conditions

$$\vec{v}^s = \vec{v}^f \quad \text{on } \Gamma^{fs} \tag{3.4.44}$$

$$\vec{u} = \vec{0} \quad \text{on } \Gamma_I \tag{3.4.45}$$

$$\vec{u} = \vec{0} \quad \text{on } \Gamma_O \tag{3.4.46}$$

$$\boldsymbol{t}^s\vec{n}^s = \vec{0} \quad \text{on } \Gamma_E^s \tag{3.4.47}$$

$$\boldsymbol{t}^s\vec{n}^s = -\boldsymbol{t}^f\vec{n}^f \quad \text{on } \Gamma^{fs} \tag{3.4.48}$$

$$\vec{v} = \vec{0} \quad \text{on } \Gamma_I^s \tag{3.4.49}$$

$$\vec{v} = \vec{0} \quad \text{on } \Gamma_O^s \tag{3.4.50}$$

$$\vec{v} = \vec{v}_I \quad \text{on } \Gamma_I^f \tag{3.4.51}$$

$$\frac{\partial \vec{v}}{\partial \vec{n}} = 0 \quad \text{on } \Gamma_O^f. \tag{3.4.52}$$

We have prescribed velocity on the input and on the output. There is a free boundary condition. The various boundary conditions for velocity on input and output are discussed in the next chapter.

3.5 Fluid Constitutive Relations

For the fluid part we only prescribe incompressible Newtonian fluid

$$\boldsymbol{t}^f = -p^f \boldsymbol{I} + \mu \left(\nabla \vec{v}^f + \nabla^T \vec{v}^f \right). \tag{3.5.53}$$

3.6 Constitutive Relations for Elastic Material

We promised the total derivation of $\boldsymbol{P}$ under the assumptions of isotermicity and incompressibility. The results follow.

3.6.1 *The First Piola-Kirchhoff pseudo-stress tensor*

3.6.1.1 *Helmholtz potential* A very common method of prescribing constitutive relations lies in the specification of free energy or Helmholtz potential Ψ. We have to use some thermodynamic basics:

Internal energy can be expressed by using the thermodynamic potential as

$$\varepsilon = \Psi + Ts,$$

where s is entropy and T temperature.

It is obvious, that any constitutive relation must correspond to the 1st and 2nd Thermodynamic Laws, where the 2nd can be represented by

Theorem 3.3 (Clausius-Duhem inequality).

$$\Sigma(S) = \rho_0 \dot{s} + \frac{\partial}{\partial X^K} \left(\frac{Q^K}{T} \right) - \frac{\tilde{Q}}{T} \geq 0 \tag{3.6.54}$$

or equivalently

$$-\rho_0 \left(\frac{d\Psi}{dt} + s \frac{dT}{dt} \right) + \boldsymbol{P}^T \frac{d\boldsymbol{F}}{dt} - \frac{1}{T} Q \operatorname{Div} T \geq 0. \tag{3.6.55}$$

For our purposes, the second formula will be very important. We exclude heat fluxes, due to the isotermicity assumption,

$$-\rho_0 \frac{d\Psi}{dt} + \boldsymbol{P}^T \frac{d\boldsymbol{F}}{dt} \geq 0. \tag{3.6.56}$$

The equipressential axiom ensures that $\boldsymbol{P}$ and Ψ depend on all state quantities. Using our assumption of isotermicity and disregarding heat fluxes, both quantities depend on the components of $\boldsymbol{F}$.

Now we assume only elastic deformation (there will be an equality in 3.3 and in 3.6.56) and we use the dependence of $\boldsymbol{P}$ on the components of $\boldsymbol{F}$ in the derivative

$$\frac{d\Psi}{dt} = \frac{\partial \Psi}{\partial \boldsymbol{F}} \frac{d\boldsymbol{F}}{dt},$$

which results in

$$\left(-\rho_0 \frac{\partial \Psi}{\partial \boldsymbol{F}} + \boldsymbol{P}^T \right) \frac{d\boldsymbol{F}}{dt} = 0 \quad \forall \boldsymbol{F}.$$

Because of the free choice of $\boldsymbol{F}$, it is clear, that the term in brackets must be identically equal to zero. We expressed $\boldsymbol{P}$ with respect to Ψ

$$\boldsymbol{P} = \rho_0 \frac{\partial \Psi}{\partial \boldsymbol{F}^T}.$$

3.6.1.2 *Stress Energy* We have shown that $\Psi = \Psi(\boldsymbol{F})$, which we can use for the description of the isothermal elastic deformation of a homogeneous body. Using the 1st Thermodynamic Law we can easily show, that for isothermal processes the stress energy W per unit mass is

$$\varrho_0 \Psi(\boldsymbol{F}) = W(\boldsymbol{F}). \tag{3.6.57}$$

3.6.1.3 *Properties of* Ψ It is natural to omit the dependence of Ψ on motion. We can do this using the decomposition of the deformation gradient

$$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U}, \qquad \boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F} = \boldsymbol{U}^2 \text{ so } \Psi = \Psi(\boldsymbol{C}),$$

where $\boldsymbol{R}$ is pure rotation and $\boldsymbol{U}$ is displacement. It remains to derive

$$\frac{\partial \Psi}{\partial \boldsymbol{F}^T} = 2\frac{\partial \Psi}{\partial \boldsymbol{C}}\boldsymbol{F}^T, \text{ hence } \quad \boldsymbol{P} = 2\frac{\partial W}{\partial \boldsymbol{C}}\boldsymbol{F}^T.$$

The last assumption, which helps us to specify the final form of the constitutive relation, is incompressibility. Assume $\det \boldsymbol{F} = 1$ and therefore $\det \boldsymbol{C} = 1$. We introduce p as the Lagrange multiplier. We get the following dependence

$$\tilde{\Psi} = \Psi(\boldsymbol{F}) - p(\det \boldsymbol{F} - 1),$$

and in 3.6.56 we get

$$\left(-\rho_0 \frac{\partial \Psi}{\partial \boldsymbol{F}} + \rho_0 p j \boldsymbol{F}^{-T} + \boldsymbol{P}^T\right) \frac{d\boldsymbol{F}}{dt} + \rho_0 (j-1) \frac{dp}{dt} = 0 \qquad \forall (\boldsymbol{F}, p).$$

Because $\boldsymbol{F}$ and p are chosen arbitrarily, we get

$$\boxed{\boldsymbol{P} = \rho_0 \left(\frac{\partial \Psi}{\partial \boldsymbol{F}^T} - jp\boldsymbol{F}^{-1}\right), \qquad j = 1}.$$

3.6.1.4 *Application to constitutive relations* Now we have to take care of $\frac{\partial \Psi}{\partial \mathbf{F}}$, which is in the balance of linear momentum in the form of $\operatorname{Div} \boldsymbol{P}^T$. Using the facts in the last paragraph we can write

$$\boldsymbol{P}^T = \rho_0 \left(\frac{\partial \Psi}{\partial \boldsymbol{F}} - p\boldsymbol{F}^{-T}\right) = -jp\boldsymbol{F}^{-T} + j\rho \frac{\partial \Psi}{\partial \boldsymbol{F}} = -jp\boldsymbol{F}^{-T} + 2j\boldsymbol{F}\frac{\partial W}{\partial \boldsymbol{C}},$$

where ϱ_0 was absorbed into the pressure p.

In the main constitutive relations it remains to specify W and compute $\frac{\partial W}{\partial \mathbf{C}}$. For example if we use the Mooney-Rivlin material, and we use simplified 3.3.37, we obtain

$$W = c_1 (I_C - 3) + c_2 (II_C - 3).$$

For the computation of the derivative term $\frac{\partial W}{\partial \mathbf{C}}$ we use the Caley-Hamilton theorem (tensor fulfils its own characteristic polynom)

$$-\boldsymbol{C}^3 + I_C\boldsymbol{C}^2 - II_C\boldsymbol{C} + III_C\boldsymbol{I} = 0. \tag{3.6.58}$$

If we multiply 3.6.58 by $\boldsymbol{C}^{-1}$ and apply the trace operator tr, we get

$$\operatorname{tr}(\boldsymbol{C}^2) - I_C \operatorname{tr}(\boldsymbol{C}) + II_C \operatorname{tr}(\boldsymbol{I}) = III_C \operatorname{tr}(\boldsymbol{C}^{-1}).$$

Therefore, (using the definition of the second invariant), it is obvious that

$$\operatorname{tr}(\boldsymbol{C}^{-1}) = \frac{II_C}{III_C}.$$

If we now differentiate 3.6.58 with respect to $\boldsymbol{C}$ and use the definitions of tensor's invariants, we get the following formulas

$$\frac{\partial I_C}{\partial \mathbf{C}} = \boldsymbol{I} \tag{3.6.59}$$

$$\frac{\partial II_C}{\partial \mathbf{C}} = I_C\boldsymbol{I} - \boldsymbol{C}^T \tag{3.6.60}$$

$$\frac{\partial III_C}{\partial \mathbf{C}} = III_C\boldsymbol{C}^{-T} \tag{3.6.61}$$

We are interested in the $\frac{\partial W}{\partial \mathbf{C}}$ term, but this is very simple now

$$\frac{\partial W}{\partial \boldsymbol{C}} = c_1\boldsymbol{I} + c_2 \operatorname{tr}(\boldsymbol{C})\boldsymbol{I} - c_2\boldsymbol{C}.$$

MATHEMATICAL PROBLEM FORMULATION

Now we have to formulate our problem more precisely from the mathematical point of view. We wish to prepare it for numerical computations, so we will start with the classical formulation. Then we will prepare the dimensionless version and at the end we will introduce the weak formulation.

We recall equations from last chapter, but for brevity we change notation from Cartesian components to vector.

4.1 Classical formulation

4.1.1 *Model equations*

We take *Newtonian* fluid and *elastic* material and then the main problem will be formulated as follows :

Problem 4.1. *Find* $\vec{u}$,$\vec{v}$,p^s,p^f *to satisfy*

$$\frac{\partial \vec{u}}{\partial t} = \begin{cases} \vec{v} & in\ \Omega^s \\ \triangle \vec{u} & in\ \Omega^f \end{cases}$$

$$0 = \begin{cases} \frac{d}{dt}(\rho^s j) & in\ \Omega^s \\ \frac{\partial}{\partial t}(\rho^f j) + \mathrm{Div}\left(\rho^f j(\vec{v} - \frac{\partial \vec{u}}{\partial t})\boldsymbol{F}^{-T}\right) & in\ \Omega^f \end{cases}$$

$$\frac{\partial \vec{v}}{\partial t} = \begin{cases} \frac{1}{j\rho^s}\,\mathrm{Div}\,\boldsymbol{P}^{sT} - \vec{\mathcal{F}} & in\ \Omega^s \\ -(\nabla \vec{v})(\vec{v} - \frac{\partial \vec{u}}{\partial t})\boldsymbol{F}^{-T} + \frac{1}{j\rho^f}\,\mathrm{Div}(j\boldsymbol{t}^f\boldsymbol{F}^{-T}) - \vec{\mathcal{F}} & in\ \Omega^f \end{cases}$$

with initial conditions

$$\begin{aligned} \vec{u}(0) &= \vec{0} \qquad in\ \Omega, \\ \vec{v}(0) &= \vec{v}_0 \qquad in\ \Omega, \end{aligned}$$

and boundary conditions

$$\begin{aligned} \vec{v} &= \vec{v}_I \qquad on\ \Gamma_I^f, \\ \vec{u} &= \vec{0} \qquad on\ \Gamma_I,\ \Gamma_O, \\ \vec{v} &= \vec{0} \qquad on\ \Gamma_I^s,\ \Gamma_O^s, \\ \frac{\partial \vec{v}}{\partial \vec{n}} &= \vec{0} \qquad on\ \Gamma_O^f, \\ \boldsymbol{t}^s\vec{n} &= \vec{0} \qquad on\ \Gamma_E, \end{aligned}$$

with constitutive relations

$$\boldsymbol{t}^f = -p^f \boldsymbol{I} + \mu \left(\nabla \vec{v} + \nabla^T \vec{v}\right),$$
$$\boldsymbol{P}^{sT} = -jp^s \boldsymbol{F}^{-T} + 2j\boldsymbol{F}\frac{\partial W}{\partial \boldsymbol{C}}.$$

Remark 4.2 (About fluid constitutive relations). *Stress tensor t^f, which we prescribed, must be transformed into reference configuration and simplified using* $\operatorname{div} \vec{v} = \vec{0}$. *We write*

$$\begin{aligned}\operatorname{Div}(j\boldsymbol{t}^f \boldsymbol{F}^{-T}) &= \operatorname{Div}\left(-jp^f \boldsymbol{F}^{-T} + j\mu\left(\nabla\vec{v} + \nabla\vec{v}^T\right)\boldsymbol{F}^{-1}\boldsymbol{F}^{-T}\right)\\ &= \operatorname{Div}\left(-jp^f \boldsymbol{F}^{-T}\right) + \operatorname{Div}\left(j\mu\nabla\vec{v}\boldsymbol{F}^{-1}\boldsymbol{F}^{-T}\right)\\ &+ \underline{\operatorname{Div}\left(j\mu\nabla^T\vec{v}\boldsymbol{F}^{-1}\boldsymbol{F}^{-T}\right)},\end{aligned}$$

where the underlined term vanishes, because of

$$\frac{\partial}{x_j}\left(\frac{\partial v_j}{\partial x_i}\right) = \frac{\partial}{\partial x_i}(\underbrace{\operatorname{div}\vec{v}}_{0}).$$

4.1.2 *Dimensionless formulation*

For numeric computation it is suitable to reformulate our problem to a dimensionaless formulation. You can easily imagine, that to compute i.e. $\sin(10\,kg)$ is not possible. Therefore we introduce the characteristic length L^* and velocity $\vec{V}^*$. We multiply all quantities by their characteristic versions. When we need to multiply by density, we choose ϱ^f. We arrive to the following formulas

$$\begin{aligned}\vec{v}' &= \vec{v}\frac{1}{V^*} & \vec{x}' &= \vec{x}\frac{1}{L^*}\\ \vec{u}' &= \frac{\vec{u}}{L^*}\\ p' &= p\frac{1}{V^{*2}} & t' &= t\frac{V^*}{L^*}\\ \boldsymbol{t}^{s\prime} &= \boldsymbol{t}^s\frac{1}{\rho^f V^{*2}} & \beta &= \tfrac{\rho^s}{\rho^f}\\ \mu' &= \mu\frac{1}{\rho^f V^* L^*} & W' &= W\frac{1}{\rho^f V^{*2}}.\end{aligned}$$

Now we must compute all quantities without primes and substitute them into Problem 4.1. It is practical to denote primed quantities as non primed.

After that we have a new

Problem 4.3. *Find $\vec{u}$,$\vec{v}$,p^s,p^f to satisfy the following:*

Equations relevant to Ω^s :

$$\frac{\partial \vec{u}}{\partial t} = \vec{v} \tag{4.1.1}$$
$$0 = j - 1 \tag{4.1.2}$$
$$\frac{\partial \vec{v}}{\partial t} = \frac{1}{\beta j}\operatorname{Div}\left(-jp^s \boldsymbol{F}^{-T} + 2j\boldsymbol{F}\frac{\partial W}{\partial \boldsymbol{C}}\right) - \vec{\mathcal{F}} \tag{4.1.3}$$

Equations relevant to Ω^f *:*

$$\frac{\partial \vec{u}}{\partial t} = \triangle \vec{u} \tag{4.1.4}$$

$$\vec{0} = \mathrm{Div}\left(j\vec{v}\boldsymbol{F}^{-T}\right) \tag{4.1.5}$$

$$\frac{\partial \vec{v}}{\partial t} = -\nabla v\left(\boldsymbol{F}^{-1}\right)\left(\vec{v} - \frac{\partial \vec{u}}{\partial t}\right) \tag{4.1.6}$$

$$+\frac{1}{j}\,\mathrm{Div}\left(-jp^f\boldsymbol{F}^{-T} + j\mu\nabla\vec{v}\boldsymbol{F}^{-1}\boldsymbol{F}^{-T}\right) - \vec{\mathcal{F}}$$

with initial and boundary conditions from Problem 4.1

4.2 Weak formulation

We multiply equations in Problem 4.3 by test functions $\vec{\varsigma}$,η,$\vec{\xi}$, integrate over the domain Ω and over the time interval $[0,T]$. We use the Green theorem on some terms. For the correctness of integral forms we will assume $\frac{\partial \vec{u}}{\partial t} \in L^2\left([0,T]\times\Omega\right)$ and assume external forces $\vec{\mathcal{F}}$ has to be from $L^2\left(0,T;[W^{-1,2}]^3\right)$.

For the formulation of the problem corresponding to Problem 4.3 we need to specify properties of test functions $\vec{\varsigma}$ and $\vec{\xi}$ with respect to the boundary. We prescribe $\vec{\varsigma} = \vec{0}$ on Γ_I,Γ_O and $\vec{\xi} = \vec{0}$ on Γ_I and Γ_O^s. We provide a more precise discussion later in Chapter 4.4.

Now we integrate the equations of Problem 4.3 and we get

$$\int_0^T\int_\Omega \frac{\partial \vec{u}}{\partial t}\cdot\vec{\varsigma}\,\mathrm{dVdt} = \int_0^T\int_{\Omega^s}\vec{v}\cdot\vec{\varsigma}\,\mathrm{dVdt} - \int_0^T\int_{\Omega^f}\nabla\vec{u}\cdot\nabla\vec{\varsigma}\,\mathrm{dVdt} \tag{4.2.7}$$

$$0 = \int_0^T\int_{\Omega^s}(j-1)\cdot\eta\,\mathrm{dVdt} + \int_0^T\int_{\Omega^f}\mathrm{Div}\left(j\vec{v}\boldsymbol{F}^{-T}\right)\cdot\eta\,\mathrm{dVdt} \tag{4.2.8}$$

$$\int_0^T\left\langle j\beta\frac{\partial\vec{v}}{\partial t},\vec{\xi}\right\rangle\mathrm{dt} + \int_0^T\left\langle\frac{\partial\vec{v}}{\partial t},\vec{\xi}\right\rangle\mathrm{dt} = \tag{4.2.9}$$

$$= \int_0^T\int_\Omega jp\boldsymbol{F}^{-T}\cdot\nabla\vec{\xi}\,\mathrm{dVdt}$$

$$- \int_0^T\int_{\Omega^s} 2j\boldsymbol{F}\frac{\partial W}{\partial \boldsymbol{C}}\cdot\nabla\vec{\xi}\,\mathrm{dVdt}$$

$$- \int_0^T\int_{\Omega^f} j\nabla\vec{v}\left(\boldsymbol{F}^{-1}\right)\left(\vec{v} - \frac{\partial\vec{u}}{\partial t}\right)\cdot\vec{\xi}\,\mathrm{dVdt}$$

$$- \int_0^T\int_{\Omega^f} j\mu\nabla\vec{v}\boldsymbol{F}^{-1}F^{-T}\cdot\nabla\vec{\xi}\,\mathrm{dVdt}$$

$$- \int_0^T\left\langle j\beta\vec{\mathcal{F}},\vec{\xi}\right\rangle\mathrm{dt} - \int_0^T\left\langle j\vec{\mathcal{F}},\vec{\xi}\right\rangle\mathrm{dt}.$$

For the problem formulation we have to define the following function spaces

$$U = \{\vec{u} \in L^\infty(I, [W^{1,2}(\Omega)]^3), \vec{u} = \vec{0} \text{ on } \Gamma_I, \Gamma_O\},$$
$$P = \{p \in L^2(I, L^2(\Omega))\},$$
$$V = \{\vec{v} \in L^2(I, [W^{1,2}(\Omega_t)]^3) \cap L^\infty(I, [L^2(\Omega_t)]^3), \vec{v} = \vec{0} \text{ on } \Gamma_I, \Gamma_O^s\}$$

and have to define the space for test functions

$$\mathcal{T} = C^\infty([0, T] \times \Omega).$$

For the energy estimates, which are required for the spaces definitions, please see (Hron, 2001).

Now we have everything ready for variational problem formulation.

Problem 4.4. *Find* $(\vec{u}, p, \vec{v} - \vec{v}_I) \in U \times P \times V$, *such that equations 4.2.7, 4.2.8, 4.2.9 are satisfied for all* $(\vec{\varsigma}, \eta, \vec{\xi}) \in [\mathcal{T}]^3 \times \mathcal{T} \times [\mathcal{T}]^3$.

4.3 What does the model remind you of?

At first glance Problem 4.4 is too complicated. But after some simplification we see, that it is nothing else than deformed Navier-Stokes. Now try to forget the interaction terms. It means $\vec{u} = \vec{0}$ and so $\boldsymbol{F} = \boldsymbol{I}$, $j = 1$. We omit 4.2.7 and see, what is left.

The equation 4.2.8 will change into

$$0 = \int_0^T \int_{\Omega f} \mathrm{Div}\,(\vec{v}) \cdot \eta \,\mathrm{dV dt}. \tag{4.3.10}$$

The equation 4.2.9 will be

$$\begin{aligned} \int_0^T \langle \frac{\partial \vec{v}}{\partial t}, \vec{\xi} \rangle \,\mathrm{dt} = & \int_0^T \int_{\Omega f} p \cdot \nabla \vec{\xi} \,\mathrm{dV dt} \\ & - \int_0^T \int_{\Omega f} (\vec{v} \cdot \nabla) \vec{v} \vec{\xi} \,\mathrm{dV dt} \\ & - \int_0^T \int_{\Omega f} \mu \nabla \vec{v} \cdot \nabla \vec{\xi} \,\mathrm{dV dt}. \end{aligned} \tag{4.3.11}$$

The system of equations 4.3.10 and 4.3.11 is the well-known Navier-Stokes. We can use a lot of techniques for solving our problem with methods normally used for NS.

4.4 Boundary Conditions

We formulated our problem for one kind of input/output boundary conditions. But there are more types, which we can prescribe. We omitted $\vec{u}$ now and we will talk only about velocity $\vec{v}^f$ and pressure p^f.

This chapter is about the possible BCs in fluid. For brevity we will talk about equations 4.3.10 and 4.3.11 instead of 4.2.8 and 4.2.9.

4.4.1 *Velocity on the input*

The velocity on the input can be prescribed using the Dirichlet boundary condition. We used this technique in our formulation. We can prescribe any values, but it is always required to relate to some physical background. We have viscous flow, therefore on solid boundary the velocity has zero value. Hence it is natural to copy this in the prescription of velocity on the input.

A well known example is Poisson's flow (see (Brdička, 2000)). We use this for a numerical experiment, which can be found in Chapter 5.3. For the flow in a tube the velocity vector field has a parabolic profile.

4.4.2 *Velocity on the output*

The velocity on the output can be prescribed in the same way as the input one. It means using the Dirichlet condition. The change for our formulation will be as follows.

In boundary conditions

$$\begin{aligned} \vec{v} &= \vec{v}_{IO} \quad \text{on } \Gamma_I \\ \vec{v} &= \vec{v}_{IO} \quad \text{on } \Gamma_O, \end{aligned}$$

where $\vec{v}_{IO}$ is defined as

$$\vec{v}_{IO} = \begin{cases} \vec{v}_I & \text{on } \Gamma_I \\ \vec{v}_O & \text{on } \Gamma_O. \end{cases}$$

In the definition of function spaces

$$V = \{\vec{v} \in L^2(I, [W^{1,2}(\Omega_t)]^3) \cap L^\infty(I, [L^2(\Omega_t)]^3), \vec{v} = \vec{0} \text{ on } \Gamma_I, \Gamma_O\}.$$

And in the variational formulation
Find $(\vec{u}, p, \vec{v} - \vec{v}_{IO}) \in U \times P \times V$.

In our formulation we used a different type of BC. It is called the free boundary prescription and it is represented by Neumann condition. It means the prescription of behavior of velocity derivative with respect to the outer normal. If we prescribe zero value, it means no change in the outer direction - free outflow.

Now we take care about this condition in greater detail. If we change from classical formulation into variational, we need to use the Green formula it the following way

$$\begin{aligned} &\int_\Omega (-\mu \triangle \vec{v} + \nabla p + (\vec{v} \cdot \nabla)\vec{v}) \cdot \vec{\xi}\, dv = \\ &= \int_{\Gamma_O} \left(p\vec{n} - \mu \frac{\partial \vec{v}}{\partial \vec{n}} \right) \cdot \vec{\xi} d\Gamma + \int_\Omega \nabla \vec{v} \cdot \nabla \vec{\xi} - p \operatorname{div} \vec{\xi} + (\vec{v} \cdot \nabla)\vec{v} \cdot \vec{\xi}\, dv, \end{aligned}$$

where the boundary condition is

$$p\vec{n} - \mu \frac{\partial \vec{v}}{\partial \vec{n}} = 0. \tag{4.4.12}$$

4.4.3 *Flow by pressure gradient*

But there is another way how to start the motion in a tube. We will not prescribe velocity on input nor output. Look carefully on condition 4.4.12. If we imagine the term $\frac{\partial \vec{v}}{\partial \vec{n}} = 0$, we can prescribe pressure p on the boundary. If we prescribe higher value of pressure on input and lower value on output the flow starts in the direction of the pressure gradient.

Changes in the formulation will be as follows.

In the boundary conditions

$$p\vec{n} - \mu \frac{\partial \vec{v}}{\partial \vec{n}} = 0.$$

In function spaces definition

$$V = \{\vec{v} \in L^2(I, [W^{1,2}(\Omega_t)]^3) \cap L^\infty(I, [L^2(\Omega_t)]^3)\}.$$

And in variational formulation

Find $(\vec{u},p,\vec{v}) \in U \times P \times V$.

NUMERICAL METHOD

The main target of this work are numerical experiments based on Problem 4.4. For this we must discretize the problem. The discretization will be in time and in space. To obtain the solution we wrote a program, which is algorithmicaly equivalent to the numerical method described below. We also need space description - the meshes. At the end of the chapter we give simple a paragraph about getting meshes for fluid-structure interaction problems.

5.1 Problem Discretization

We start with time discretization and then we formulate space discretization using the FEM method.

5.1.1 *Time discretization*

For the time discretization we use the implicit Euler method and semi implicit Crank-Nicholson method. We use the Crank-Nicholson method for the main computations but it has a disadvantage: it is only conditionally stable.

We have the time interval $(0, T)$. We divide it into n subintervals $I_n = [t^n, t^{n+1}]$ with constant time step $k_n = t^{n+1} - t^n$.

Remark 5.1 (About notation). *With superscript ^{n} we denote the quantity on time level t^n.*

We rewrite Problem 4.4 for the time interval $[t^n, t^{n+1}]$ and we approximate the time derivation $\frac{\partial f}{\partial t}$ by central differences,

$$\frac{\partial f}{\partial t} \approx \frac{f^{n+1} - f^n}{k_n}$$

or by higher order

$$\frac{\partial f}{\partial t} \approx \frac{3f^{n+1} - 4f^n + f^{n-1}}{2k_n}.$$

We approximate time integrals using the Newton-Cotes formulas, especially by the trapezoidal rule ($\theta = \frac{1}{2}$)

$$\int_{t^n}^{t^{n+1}} f \,\mathrm{dt} \approx (t^{n+1} - t^n) \left\{ \theta\, f(t^{n+1}) + (1 - \theta)\, f(t^n) \right\}.$$

Remark 5.2 (Notation).

$F^n = I + \nabla u^n$ $\qquad$ $j^n = \det F^n$

$(a, b)_f = \int_{\Omega_f} a \cdot b \,\mathrm{dV}$ $\qquad$ $(a, b)_s = \int_{\Omega_s} a \cdot b \,\mathrm{dV}$ $\qquad$ $(a, b) = \int_{\Omega} a \cdot b \,\mathrm{dV}$

5.1.1.1 *Crank-Nicholson scheme* To obtain the Crank-Nicolson scheme we will put $\theta = 0.5$ into the following scheme and Problem 4.4 will take following form.

Grid deformation equation 4.2.7

$$\begin{aligned} 0 =&(\vec{u}^{n+1}, \varsigma) - (\vec{u}^{n}, \varsigma) \\ &- \theta\, k_n(\vec{v}^{n+1}, \varsigma)_s - (1-\theta) k_n(\vec{v}^{n}, \varsigma)_s \\ &+ \theta\, k_n(\nabla \vec{u}^{n+1}, \nabla \varsigma)_f + (1-\theta) k_n(\nabla \vec{u}^{n}, \nabla \varsigma)_f. \end{aligned} \tag{5.1.1}$$

We consider the continuity equation 4.2.8 implicitly to prevent numerical oscillations. This effect is known from the NS problem.

We use the Piola identity in Ω_f to rewrite $\mathrm{Div}\left(j\vec{v}\boldsymbol{F}^{-T}\right) = j\nabla\vec{v}\cdot\boldsymbol{F}^{-1}$,

$$0 = \left(j^{n+1} - 1, \eta\right)_s + \left(j^{n+1}\nabla v^{n+1}\left(F^{n+1}\right)^{-1}, \eta\right)_f. \tag{5.1.2}$$

The linear momentum equation 4.2.9

$$\begin{aligned} 0 =& \left(\beta j^{n+1}\vec{v}^{n+1}, \vec{\xi}\right)_s - \left(\beta j^{n}\vec{v}^{n}, \vec{\xi}\right)_s \\ &+ \left(j^{n+1}\vec{v}^{n+1}, \vec{\xi}\right)_f - \left(j^{n}\vec{v}^{n}, \vec{\xi}\right)_f \\ &- k_n\left(j^{n+1}p^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-T}, \nabla\vec{\xi}\right)_f - k_n\left(j^{n+1}p^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-T}, \nabla\vec{\xi}\right)_s \\ &- \theta\left(\nabla\vec{v}^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-1}\left(\vec{u}^{n+1} - \vec{u}^{n}\right), \vec{\xi}\right)_f - (1-\theta)\left(\nabla\vec{v}^{n}\left(\boldsymbol{F}^{n}\right)^{-1}\left(\vec{u}^{n+1} - \vec{u}^{n}\right), \vec{\xi}\right)_f \\ &+ \theta\, k_n\left(2j^{n+1}\boldsymbol{F}^{n+1}\frac{\partial W}{\partial \boldsymbol{C}}, \nabla\vec{\xi}\right)_s + (1-\theta)k_n\left(2j^{n}\boldsymbol{F}^{n}\frac{\partial W}{\partial \boldsymbol{C}}, \nabla\vec{\xi}\right)_s \\ &+ \theta\, k_n\left\{\begin{array}{l} \mu\left(j^{n+1}\nabla\vec{v}^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-1}\left(\boldsymbol{F}^{n+1}\right)^{-T}, \nabla\vec{\xi}\right)_f \\ + \mu\left(j^{n}\nabla\vec{v}^{n}\left(\boldsymbol{F}^{n}\right)^{-1}\left(\boldsymbol{F}^{n}\right)^{-T}, \nabla\vec{\xi}\right)_f \end{array}\right\} \\ &+ (1-\theta)k_n\left\{\left(j^{n+1}\nabla\vec{v}^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-1}v^{n+1}, \vec{\xi}\right)_f + \left(j^{n}\nabla\vec{v}^{n}\left(\boldsymbol{F}^{n}\right)^{-1}\vec{v}^{n}, \vec{\xi}\right)_f\right\} \\ &- \theta\, k_n\left(j^{n+1}\vec{\mathcal{F}}^{n+1}, \vec{\xi}\right)_f - (1-\theta)k_n\left(j^{n}\vec{\mathcal{F}}^{n}, \vec{\xi}\right)_f \\ &- \theta\, k_n\left(\beta j^{n+1}\vec{\mathcal{F}}^{n+1}, \vec{\xi}\right)_s - (1-\theta)k_n\left(\beta j^{n}\vec{\mathcal{F}}^{n}, \vec{\xi}\right)_s. \end{aligned} \tag{5.1.3}$$

5.1.1.2 *Implicit Euler scheme* The Problem 4.4 will take following form

$$0 =(u^{n+1}, \varphi) - (u^{n}, \varphi) - k_n\left\{(v^{n+1}, \varphi)_s\right\} + k_n\left\{(\nabla u^{n+1}, \nabla\varphi)_f\right\}, \tag{5.1.4}$$

$$0 = \left(j^{n+1} - 1, \eta\right)_s + \left(j^{n+1}\nabla v^{n+1}\left(F^{n+1}\right)^{-1}, \eta\right)_f, \tag{5.1.5}$$

$$
\begin{aligned}
0 = & \left(\beta j^{n+1}\vec{v}^{n+1},\vec{\xi}\right)_s - \left(\beta j^{n}\vec{v}^{n},\vec{\xi}\right)_s \qquad (5.1.6)\\
& + \left(j^{n+1}\vec{v}^{n+1},\vec{\xi}\right)_f - \left(j^{n}\vec{v}^{n},\vec{\xi}\right)_f \\
& - k_n\left(j^{n+1}p^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-T},\nabla\vec{\xi}\right)_f - k_n\left(j^{n+1}p^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-T},\nabla\vec{\xi}\right)_s \\
& - \left(\nabla\vec{v}^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-1}\left(\vec{u}^{n+1}-\vec{u}^{n}\right),\vec{\xi}\right)_f \\
& + k_n\left\{\left(2j^{n+1}\boldsymbol{F}^{n+1}\frac{\partial W}{\partial \boldsymbol{C}},\nabla\vec{\xi}\right)_s\right\} \\
& + k_n\left\{\mu\left(j^{n+1}\nabla\vec{v}^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-1}\left(\boldsymbol{F}^{n+1}\right)^{-T},\nabla\vec{\xi}\right)_f\right\} \\
& + k_n\left\{\left(j^{n+1}\nabla\vec{v}^{n+1}\left(\boldsymbol{F}^{n+1}\right)^{-1}v^{n+1},\vec{\xi}\right)_f\right\} \\
& - k_n\left\{\left(j^{n+1}\vec{\mathcal{F}}^{n+1},\vec{\xi}\right)_f\right\} \\
& - k_n\left\{\left(\beta j^{n+1}\vec{\mathcal{F}}^{n+1},\vec{\xi}\right)_s\right\}.
\end{aligned}
$$

5.1.2 *Space discretization*

In the next step we will prepare the discretization in space using the **F**inite **E**lement **M**ethod. We will approximate the domain Ω by the polyhedric domain Ω_h, which can be divided into tetrahedrons. By $\mathcal{T}_h$ we will denote the set of tetrahedrons covering Ω_h. We will assume the regularity of $\mathcal{T}_h$, which means that every two elements are disjoint or have a common face, edge or point. By $\hat{T}$ we will denote the reference element (see Figure 5.1.1 for details).

The specificity of our approach is in computing the FS interaction simultaneously, in the sense of using one velocity and one displacement vector for the whole domain. Now there is the question of what kind of elements we will use for pressure, velocity and displacement. As we have written in Chapter 4.3, our system has certain similarities with the Navier-Stokes system. Therefore we will have to use a stable pair of pressure/velocity elements. The stability arguments are based on the solenoidal velocity spaces (spaces with zero divergence), which physically means incompressibility. But our solid material is incompressible too, so we can use the same kind of elements for displacement as for velocity.

One stable combination of elements on tetrahedrons is P_2, P_1. We will describe it more precisely.

5.1.2.1 P_1 *element* This element means approximation by a continuous piecewise linear function. In the words of spaces it will be

$$
\begin{aligned}
P_h &= \{\underline{p}_i \in C^0(\Omega_h)^3 : \ \underline{p}_i\lceil_{K_i} \in P_1(K_i) \quad \forall K_i \in \mathcal{T}_h\}\\
P_h &= \operatorname{span}\{\underline{p}_1,\ldots,\underline{p}_n\}, \quad \dim \vec{P}_h = n \quad \text{, where } n \text{ is the number of vertices.}
\end{aligned}
$$

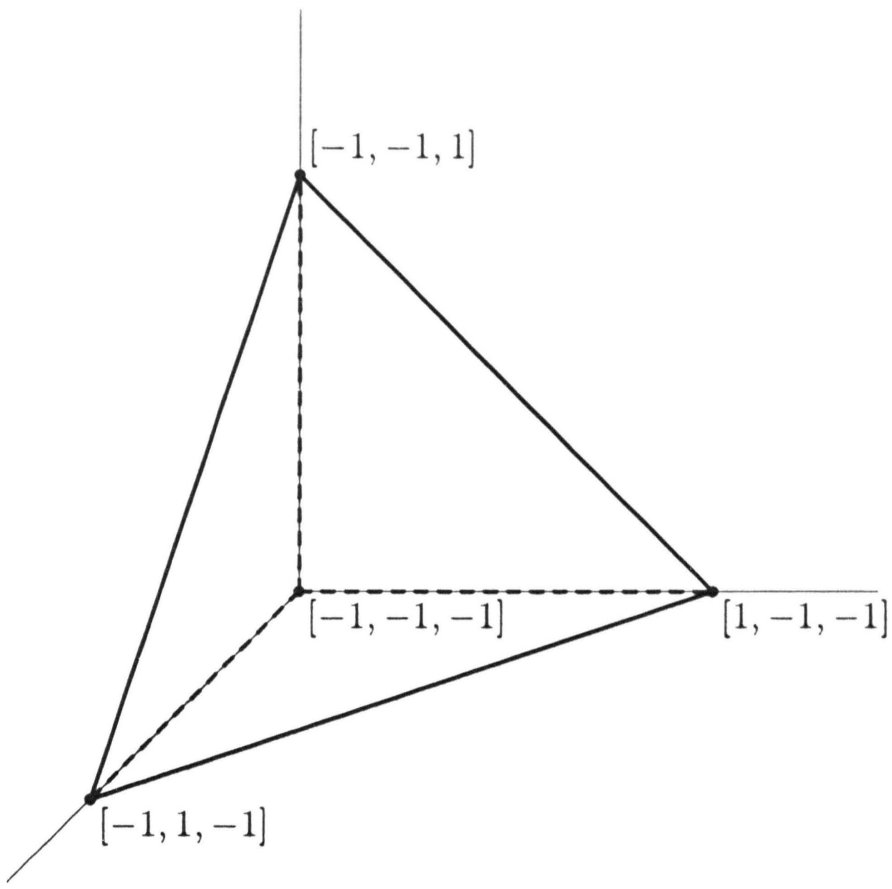


FIG. 5.1.1. Referential element $\hat{T}$

If we use $\underline{p}_i$ as space base we can write pressure p_h as

$$p_h = \sum_{k=1}^{n} d_k \underline{p}_k.$$

We will use the affine equivalence for practical computation. The local basis on the reference element can be derived from barycentrical coordinates (in this case the base functions are barycentrical coordinates - we will denote them by λ_i).

$$\begin{aligned}
f_1(\vec{x}) &= \lambda_1(\vec{x}) = -\frac{x_1 + x_2 + x_3 + 1}{2} \\
f_2(\vec{x}) &= \lambda_2(\vec{x}) = \frac{x_1 + 1}{2} \\
f_3(\vec{x}) &= \lambda_3(\vec{x}) = \frac{x_2 + 1}{2} \\
f_4(\vec{x}) &= \lambda_4(\vec{x}) = \frac{x_3 + 1}{2}
\end{aligned}$$

5.1.2.2 *P_2 element* In this case the approximation will by done by a second order polynom on each element.

$$\vec{V}_h = \{\underline{\vec{v}}_i \in [C^1(\Omega_h)]^3; \underline{\vec{v}}_i\lceil_{K_i} \in [P_2(K_i)]^3 \quad \forall K_i \in T_h\}$$
$$W_h = \text{span}\{w_1, \ldots, w_n\} \quad w_i(Q_j) = \delta_{ij}$$
$$\dim W_h = n, \text{ where } n \text{ is the number of vertices}$$
$$\vec{V}_h = \text{span}\{\underbrace{(w_1, 0, 0)}_{\underline{\vec{v}}_1}, \underbrace{(0, w_1, 0)}_{\underline{\vec{v}}_2}, \underbrace{(0, 0, w_1)}_{\underline{\vec{v}}_3}, \ldots, (0, 0, w_n), \underline{\vec{v}}_{3n+1}, \ldots, \underline{\vec{v}}_m\}$$
$$\dim \vec{V}_h = m$$
$$\underline{\vec{v}}_i \ldots \text{correspond to vertices} \quad i \leq 3n$$
$$\underline{\vec{v}}_i \ldots \text{correspond to mid-edges} \quad 3n < i \leq m$$

The velocity $\vec{v}_h$ can be written in the basis $\underline{\vec{v}}_h$ as

$$\vec{v}_h = \sum_{k=1}^{m} c_k \underline{\vec{v}}_h \tag{5.1.7}$$

and the displacement in a similar way

$$\vec{u}_h = \sum_{k=1}^{m} b_k \underline{\vec{u}}_h. \tag{5.1.8}$$

The local form of base functions can be derived from barycentrical coordinates, too.

$$\begin{aligned}
f_1(\vec{x}) &= \lambda_1(\vec{x})(2\lambda_1(\vec{x}) - 1) \\
f_2(\vec{x}) &= \lambda_2(\vec{x})(2\lambda_2(\vec{x}) - 1) \\
f_3(\vec{x}) &= \lambda_3(\vec{x})(2\lambda_3(\vec{x}) - 1) \\
f_4(\vec{x}) &= \lambda_4(\vec{x})(2\lambda_4(\vec{x}) - 1) \\
f_5(\vec{x}) &= 4\lambda_1(\vec{x})\lambda_2(\vec{x}) \\
f_6(\vec{x}) &= 4\lambda_2(\vec{x})\lambda_3(\vec{x}) \\
f_7(\vec{x}) &= 4\lambda_3(\vec{x})\lambda_1(\vec{x}) \\
f_8(\vec{x}) &= 4\lambda_1(\vec{x})\lambda_4(\vec{x}) \\
f_9(\vec{x}) &= 4\lambda_2(\vec{x})\lambda_4(\vec{x}) \\
f_{10}(\vec{x}) &= 4\lambda_3(\vec{x})\lambda_4(\vec{x})
\end{aligned}$$

Look at Fig 5.1.2 for better space view.

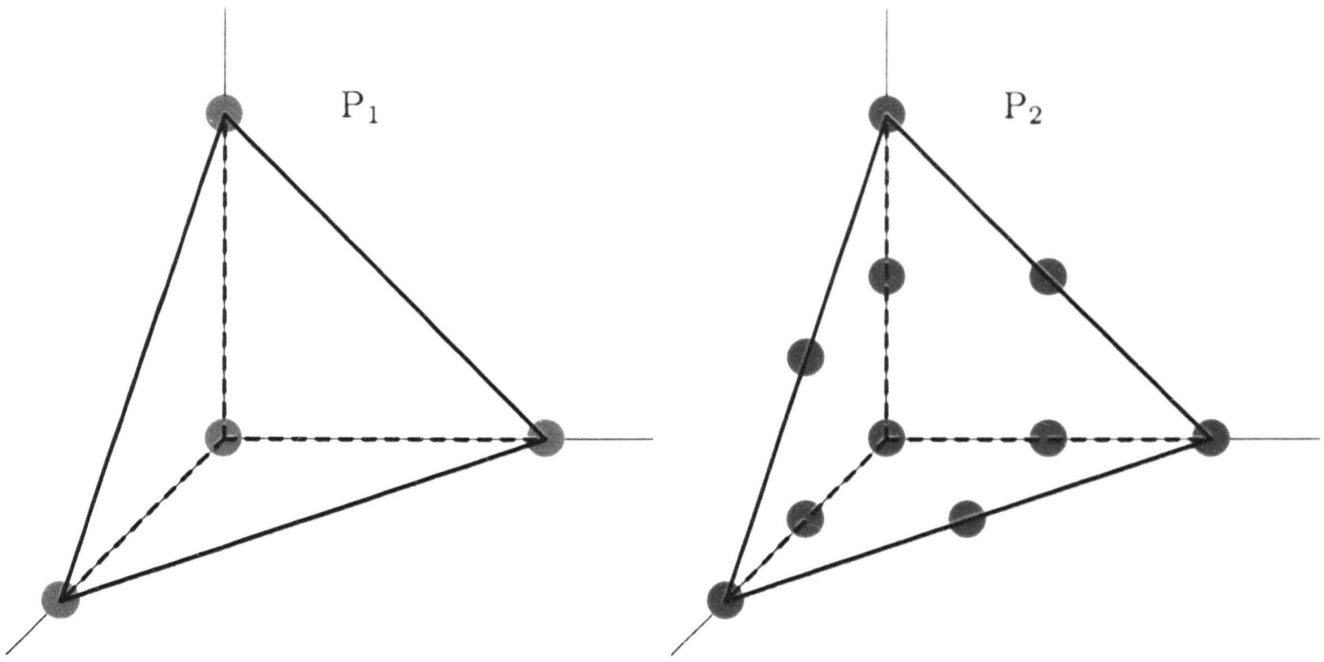


FIG. 5.1.2. Degrees of freedom for P_1,P_2

5.1.2.3 *Minielement* Another stable pair of element spaces is sometimes called *minielement*. It is continuous P_1 pressure and linear velocity with bubble function. The local basis follows

$$f_1(\vec{x}) = \lambda_1(\vec{x}) = -\frac{x_1 + x_2 + x_3 + 1}{2}$$
$$f_2(\vec{x}) = \lambda_2(\vec{x}) = \frac{x_1 + 1}{2}$$
$$f_3(\vec{x}) = \lambda_3(\vec{x}) = \frac{x_2 + 1}{2}$$
$$f_4(\vec{x}) = \lambda_4(\vec{x}) = \frac{x_3 + 1}{2}$$
$$f_5(\vec{x}) = \lambda_1(\vec{x})\lambda_2(\vec{x})\lambda_3(\vec{x})\lambda_4(\vec{x}).$$

After time discretization we have to solve the problem on each time level. We will approximate the spaces V,P,U on the time interval $[t^n, t^{n+1}]$ in the case of the P_1,P_2 pair

$$\vec{V}_h = \{\underline{\vec{v}}_h \in [C^1(\Omega_h)]^3 : \underline{\vec{v}}_h\lceil_{K_i} \in [P_2(K_i)]^3 \quad \forall K_i \in \mathcal{T}_h, \underline{\vec{v}}_h = \vec{0} \text{ on } \Gamma_I, \Gamma_O^s\}$$
$$P_h = \{\underline{p}_i \in C^0(\Omega_h) : \underline{p}_i\lceil_{K_i} \in P_1(K_i) \quad \forall K_i \in \mathcal{T}_h\}$$
$$\vec{U}_h = \{\underline{\vec{u}}_h \in [C^1(\Omega_h)]^3 : \underline{\vec{u}}_h\lceil_{K_i} \in [P_2(K_i)]^3 \quad \forall K_i \in \mathcal{T}_h, \underline{\vec{u}}_h = \vec{0} \text{ on } \Gamma_I, \Gamma_O\}.$$

Let us denote by $\vec{v}_h^n$ the approximation of $\vec{v}(t_n)$, similarly by $\vec{u}_h^n$ the approximation of $\vec{u}(t_n)$ and finally by p_h^n the approximation of $p(t_n)$.

Remark 5.3 (Notation).

$$F^n = I + \nabla \vec{u}_h^n \qquad j^n = \det F^n$$

We will insert the basis $\underline{\vec{v}}_h, \underline{p}, \underline{\vec{u}}_h$ into 5.1.1,5.1.2,5.1.3 as test functions and obtain a nonlinear algebraic set of equations

$$
\begin{aligned}
0 =&(\vec{u}_h^{n+1}, \underline{\vec{u}}_h) - (\vec{u}_h^{n}, \underline{\vec{u}}_h) \\
&- \theta\, k_n \left\{ (\vec{v}_h^{n+1}, \underline{\vec{u}}_h)_s \right\} - (1-\theta) k_n \left\{ (\vec{v}_h^{n}, \underline{\vec{u}}_h)_s \right\} \\
&+ \theta\, k_n \left\{ (\nabla \vec{u}_h^{n+1}, \nabla \underline{\vec{u}}_h)_f \right\} + (1-\theta) \left\{ (\nabla \vec{u}_h^{n}, \nabla \underline{\vec{u}}_h)_f, \right\}
\end{aligned} \tag{5.1.9}
$$

$$
0 = \left(j^{n+1} - 1, \underline{p}_h \right)_s + \left(j^{n+1} \nabla \vec{v}_h^{n+1} \left(F^{n+1} \right)^{-1}, \underline{p}_h \right)_f, \tag{5.1.10}
$$

$$
\begin{aligned}
0 =& \left(\beta j^{n+1} \vec{v}_h^{n+1}, \underline{\vec{v}}_h \right)_s - \left(\beta j^{n} \vec{v}_h^{n}, \underline{\vec{v}}_h \right)_s \\
&+ \left(j^{n+1} \vec{v}_h^{n+1}, \underline{\vec{v}}_h \right)_f - \left(j^{n} \vec{v}_h^{n}, \underline{\vec{v}}_h \right)_f \\
&- k_n \left(j^{n+1} p_h^{n+1} \left(\boldsymbol{F}^{n+1} \right)^{-T}, \nabla \underline{\vec{v}}_h \right)_f - k_n \left(j^{n+1} p_h^{n+1} \left(\boldsymbol{F}^{n+1} \right)^{-T}, \nabla \underline{\vec{v}}_h \right)_s \\
&- \theta \left(\nabla \vec{v}_h^{n+1} \left(\boldsymbol{F}^{n+1} \right)^{-1} \left(\vec{u}_h^{n+1} - \vec{u}_h^{n} \right), \underline{\vec{v}}_h \right)_f \\
&- (1-\theta) \left(\nabla \vec{v}_h^{n} \left(\boldsymbol{F}^{n} \right)^{-1} \left(\vec{u}_h^{n+1} - \vec{u}_h^{n} \right), \underline{\vec{v}}_h \right)_f \\
&+ \theta \left\{ \left(2 j^{n+1} \boldsymbol{F}^{n+1} \frac{\partial W}{\partial \boldsymbol{C}}, \nabla \underline{\vec{v}}_h \right)_s \right\} + (1-\theta) k_n \left\{ \left(2 j^{n} \boldsymbol{F}^{n} \frac{\partial W}{\partial \boldsymbol{C}}, \nabla \underline{\vec{v}}_h \right)_s \right\} \\
&+ \theta \left\{ \begin{array}{l} \mu \left(j^{n+1} \nabla \vec{v}_h^{n+1} \left(\boldsymbol{F}^{n+1} \right)^{-1} \left(\boldsymbol{F}^{n+1} \right)^{-T}, \nabla \underline{\vec{v}}_h \right)_f \\ + \mu \left(j^{n} \nabla \vec{v}_h^{n} \left(\boldsymbol{F}^{n} \right)^{-1} \left(\boldsymbol{F}^{n} \right)^{-T}, \nabla \underline{\vec{v}}_h \right)_f \end{array} \right\} \\
&+ (1-\theta) k_n \left\{ \left(j^{n+1} \nabla \vec{v}_h^{n+1} \left(\boldsymbol{F}^{n+1} \right)^{-1} v_h^{n+1}, \underline{\vec{v}}_h \right)_f + \left(j^{n} \nabla \vec{v}_h^{n} \left(\boldsymbol{F}^{n} \right)^{-1} \vec{v}_h^{n}, \underline{\vec{v}}_h \right)_f \right\} \\
&- \theta\, k_n \left(j^{n+1} \vec{\mathcal{F}}^{n+1}, \underline{\vec{v}}_h \right)_f - (1-\theta) k_n \left(j^{n} \vec{\mathcal{F}}^{n}, \underline{\vec{v}}_h \right)_f \\
&- \theta\, k_n \left(\beta j^{n+1} \vec{\mathcal{F}}^{n+1}, \underline{\vec{v}}_h \right)_s - (1-\theta) k_n \left(\beta j^{n} \vec{\mathcal{F}}^{n}, \underline{\vec{v}}_h \right)_s,
\end{aligned} \tag{5.1.11}
$$

where $\vec{v}_h$,$\vec{u}_h$ and p_h will be substituted by $\vec{v}_h = \Sigma \alpha^i \underline{\vec{v}}_h^i$, $\vec{u}_h = \Sigma \iota^j \underline{\vec{u}}_h^j$ and $p_h = \Sigma \kappa^k \underline{p}_h^k$.

Problem 5.4. *In each time step we will have to find* $\vec{\mathcal{X}} = (\vec{v}_h^{n+1}, \vec{u}_h^{n+1}, p_h^{n+1}) \in \vec{U}_h \times \vec{V}_h \times P_h$ *satisfying system 5.1.9, 5.1.10 and 5.1.11 - shortly*

$$
\vec{\mathcal{R}}(\vec{\mathcal{X}}) = \vec{0}. \tag{5.1.12}
$$

5.2 Nonlinear solver

We will use a method from numerical optimalisation for the solution of our nonlinear Problem 5.4. The basic task for these methods is the problem of finding a minimum of the function $F : \mathbb{R}^N \to \mathbb{R}$, but after a very simple correction can be used for the solution of nonlinear equations.

These methods can be characterized by the following algorithm:

1. Find the direction of $\vec{s}_k$ (direction of decline)
2. Find α_k (the step length) so that $\vec{\mathcal{X}}_k + \alpha_k \vec{s}_k$ is better in some sense

3. $\vec{\mathcal{X}}_{k+1} = \vec{\mathcal{X}}_k + \alpha_k \vec{s}_k$.

Iterate these steps until you find $\vec{\mathcal{X}}^*$ such that $F(\vec{\mathcal{X}}^*) \leq F(\vec{\mathcal{X}})\ \forall \vec{\mathcal{X}}$.

In the next part we will use the following notation: F is the minimalised function, $\vec{g} = \nabla F$, $\boldsymbol{G} = \nabla^2 F$.

The first step of our algorithm can be performed in various ways. For our problem we will use the *Newton method*, which is defined by

$$\vec{s}_i = -\boldsymbol{G}^{-1}(\vec{\mathcal{X}}_i)\vec{g}(\vec{\mathcal{X}}_i).$$

For details about other methods see (Lukšan, 2004).

Generally, the second step cannot be arbitrary. If it satisfies some conditions, at least local convergence can be proved.

Theorem 5.5. *The step length α_i, $i \in N$, satisfies the Wolfe condition, if there exist numbers $0 < \varepsilon_1 < 1/2$ and $\varepsilon_1 < \varepsilon_2 < 1$ such that*

$$Fi + 1 - F_i \leq \varepsilon_1 \alpha_i \vec{s}_i^T \vec{g}_i \tag{5.2.13}$$

and

$$\vec{s}_i^T \vec{g}_{i+1} > \varepsilon_2 \vec{s}_i^T \vec{g}_i. \tag{5.2.14}$$

The algorithm which can find the appropriate step length can be described by the following scheme (this method is called *Line search*):

1. choose $\alpha > 0$, $\overline{\alpha} = 0$
2. $\underline{\alpha} = \overline{\alpha}$; $\overline{\alpha} = \alpha$. If 5.2.13 and 5.2.14 are satisfied, then finish with $\alpha_i = \alpha$. If not 5.2.13 go to step number 4.
3. take α using extrapolation such that $\gamma_1 \overline{\alpha} \leq \alpha \leq \gamma_2 \overline{\alpha}$ and go to step 2.
4. choose α using interpolation such that $\beta_1(\overline{\alpha} - \underline{\alpha}) \leq (\alpha - \underline{\alpha}) \leq \beta_2(\overline{\alpha} - \underline{\alpha})$.
5. If 5.2.13 and 5.2.14 are satisfied, then finish with $\alpha_i = \alpha$. If not 5.2.13, set $\overline{\alpha} = \alpha$ and go to step number 4, else set $\underline{\alpha} = \alpha$ and go to step 4.

For interpolation in step 4 we can use the interpolation of quadratic or cubic functions. For brevity we introduce the notation $\phi(\alpha) = F(\vec{\mathcal{X}} + \alpha\vec{s})$ and $\phi\prime(\alpha) = \vec{s}^T g(\vec{\mathcal{X}} + \alpha\vec{s})$ and

$$A = \frac{\phi(\overline{\alpha}) - \phi(\underline{\alpha})}{(\overline{\alpha} - \underline{\alpha})\phi\prime(\underline{\alpha})} \qquad B = \frac{\phi\prime(\overline{\alpha})}{\phi\prime(\underline{\alpha})}$$

and

$$C = (B-1) - 2(A-1) \qquad D = (B-1) - 3(A-1).$$

Then quadratic interpolation means (using two values)

$$\alpha - \underline{\alpha} = \frac{\overline{\alpha} - \underline{\alpha}}{2(1-A)},$$

(using two derivatives)

$$\alpha - \underline{\alpha} = \frac{\overline{\alpha} - \underline{\alpha}}{1 - B},$$

cubic interpolation

$$\alpha - \underline{\alpha} = \frac{\overline{\alpha} - \underline{\alpha}}{D + \sqrt{D^2 - 3C}}.$$

Now we turn from the problem of finding the minimum of F to solving our nonlinear set of equations. Simply substitute $F = \frac{1}{2}\|\vec{\mathcal{R}}\|$, then $\vec{g} = \vec{\mathcal{R}}$ and $\boldsymbol{G} = \left[\nabla\vec{\mathcal{R}}\right]^{-1}$. We can formulate the solution algorithm for our nonlinear problem:

1. choose initial $\vec{\mathcal{X}} = \vec{\mathcal{X}}_0$
2. $\vec{s}_k = \left[\nabla\vec{\mathcal{R}}(\vec{\mathcal{X}}_k)\right]^{-1} \vec{\mathcal{R}}\left(\vec{\mathcal{X}}_k\right)$
3. find the step length α using quadratic/cubic line search
4. $\vec{\mathcal{X}}_{k+1} = \vec{\mathcal{X}}_k + \alpha_k \vec{s}_k$
5. go to step 2 until $\|\vec{\mathcal{R}}(\vec{\mathcal{X}}_{k+1})\| < \varepsilon$.

The second step actually means: solve linear problem $\boldsymbol{G}\vec{\mathcal{X}} = \vec{\mathcal{R}}^n$, where $\boldsymbol{G}$ is Jacobian matrix $\frac{\partial\vec{\mathcal{R}}}{\partial\vec{\mathcal{X}}}$. In general, there are two different ways of constructing the matrix $\boldsymbol{G}$. Analytically derive Problem 5.4 with respect to all unknowns, or use finite differences to approximate the matrix $\boldsymbol{G}$. We will use the second possibility.

The approximation of matrix $\boldsymbol{G}$ can be done column by column using the formula

$$\boldsymbol{G}(\vec{\mathcal{X}})e_i \approx \frac{\vec{\mathcal{R}}(\vec{\mathcal{X}} + \delta e_i) - \vec{\mathcal{R}}(\vec{\mathcal{X}} - \delta e_i)}{2\delta}$$

or

$$\boldsymbol{G}(\vec{\mathcal{X}})e_i \approx \frac{\vec{\mathcal{R}}(\vec{\mathcal{X}} + \delta e_i) - \vec{\mathcal{R}}(\vec{\mathcal{X}})}{\delta},$$

where $\delta = \sqrt{\varepsilon_M}$,$e_i$ are unit basis vectors in $\mathbb{R}^N$, ε_M is machine precision.

We will solve the linear problem by the GMRES method with ILU preconditioning. All algorithms described in this section are taken from PETSc library (Satish Balay *et al.*, 2001).

5.3 Mesh generation

The main aim of this chapter is to give a practical guide to the creation of the right mesh for our solver. We will need a very special one. Remember our approach: compute simultaneously fluid and structure. We will create a mesh, which must include two domains and a denoted internal boundary.

We have tried some mesh generators and we state only a few can do this. Finally we used the program Netgen (Joachim Schoberl *et al.*, 2003). This program expects CSG geometry format and has many export types. We've chosen *neutral format.*

Let us look on Geometry 5.6.

Geometry 5.6.

```
#
## normalized common carotid
#
algebraic3d

# cut cylinder by planes:

solid fincyl = cylinder ( 0, 0, 15; 0, 0, -1; 1.168 )
  and plane (0, 0, 0; 0, 0, -1)
  and plane (0, 0, 12; 0, 0, 1);
solid  fluid = cylinder ( 0, 0, 15; 0, 0, -1; 1.0 )
  and plane (0.0, 0, 0; 0, 0, -1)
  and plane (0, 0, 12; 0, 0, 1);
solid solid = fincyl and not fluid;

tlo fluid;
tlo solid;
```

This geometry corresponds to the normalized left carotid. It consists of two domains : *fluid* and *solid*, where solid is cylinder with radius 1.168 without fluid cylinder (radius 1.0). The very last two commands `tlo` make both domains included in the final mesh.

But there is a bad effect for the element pair P_1,P_2, which we will discuss now. The stability arguments for this pair are based on Theorem 5.7.

Theorem 5.7 (Babuška-Brezzi Condition).

$$\exists m > 0 : \qquad \inf_{q_h \in P_h} \sup_{v_h \in V_h} \frac{(\operatorname{div} v_h, q_h)}{\|q_h\|_{L^2(\Omega)} \|v_h\|_h} \geq m$$

.

The corollary for the P_1,P_2 pair is : there cannot exists an element having all vertices on the boundary.

The main problem with mesh generators is not in generating internal boundary and two domains, but in respecting this condition. Netgen was not able to generate a mesh satisfying such a condition. This resulted in the necessity to write our own program which scans the mesh for these elements and removes them. This removing is based on a simple idea: if we put a new vertex into the barycenter of a tetrahedron we have 4 new tetrahedrons all of which satisfy the discussed condition. See Figure 5.3.3 for a simple example.

From this point of view it is better to use *minielement*, which does not need this condition.

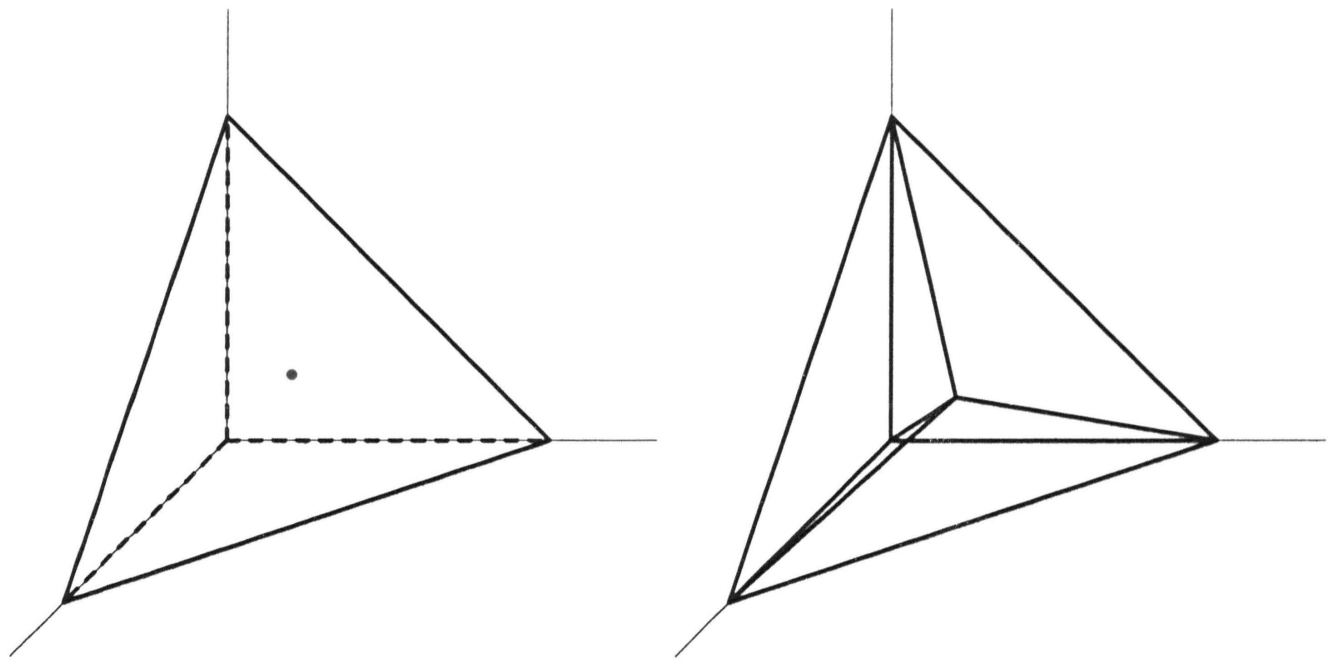


FIG. 5.3.3. Splitting tetrahedron

NUMERICAL RESULTS

A few words about numerical results. The computation in 3 space dimensions is very time and computer RAM consuming. Every result presented here was computed on computers PC with 1GB RAM and processors Pentium IV 2.8 GHz or Pentium IV HT 2.6 GHz. Every computed problem was non-stationary, so the results are animations. We highly recommend to the reader to see them on the attached CD-ROM. Each problem has its own directory under the `/problem` directory. There are static pictures, animations and a few[1] data files, which can be opened by the Mayavi program (also on CD) or by the program Tecplot. The following pictures are only static frames and cannot substitute real animation.

6.1 The Stokes problem

The simplest flow model which can be computed by our program is the Stokes problem. We can derive it by neglecting the interaction terms ($\vec{u} \equiv \vec{0}$) and the convective term in fluid ($(\vec{v}.\nabla)v \equiv \vec{0}$). The remaining linear system is very easy to solve. The results at pictures show the flow in the carotid. You can find animations of this process on the attached CD in the directory `problem/stokes`. Here we present two slides in two different times. The boundary conditions are chosen to simulate the real action which means the flow by pressure gradient. The applied pressure stroke is approximated by a sinusoidal pass of aortic pressure.

[1] We were not able to put there more data files, because the capacity of CD ROM is limited by 650 MB an we have more than 25 GB of computed data results

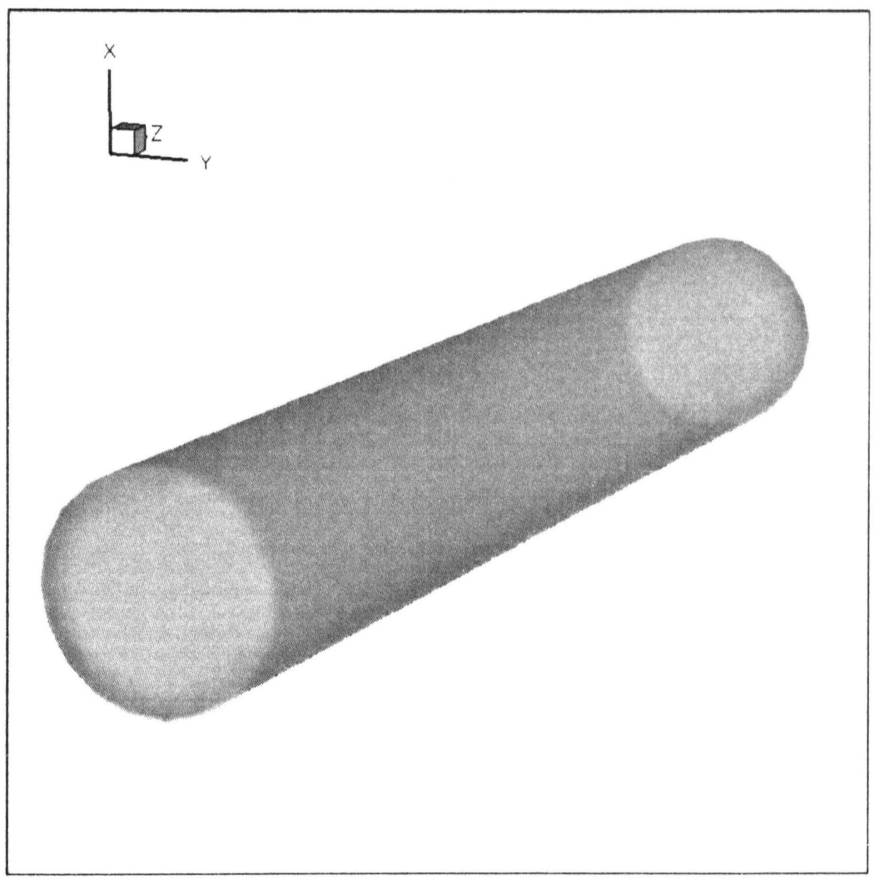


FIG. 6.1.1. Stokes problem - Carotid

Vertices	1 644
Elements	23 232
Equations	42 342
Comp time	2 hours
Time iters	98

TABLE 6.1.1.

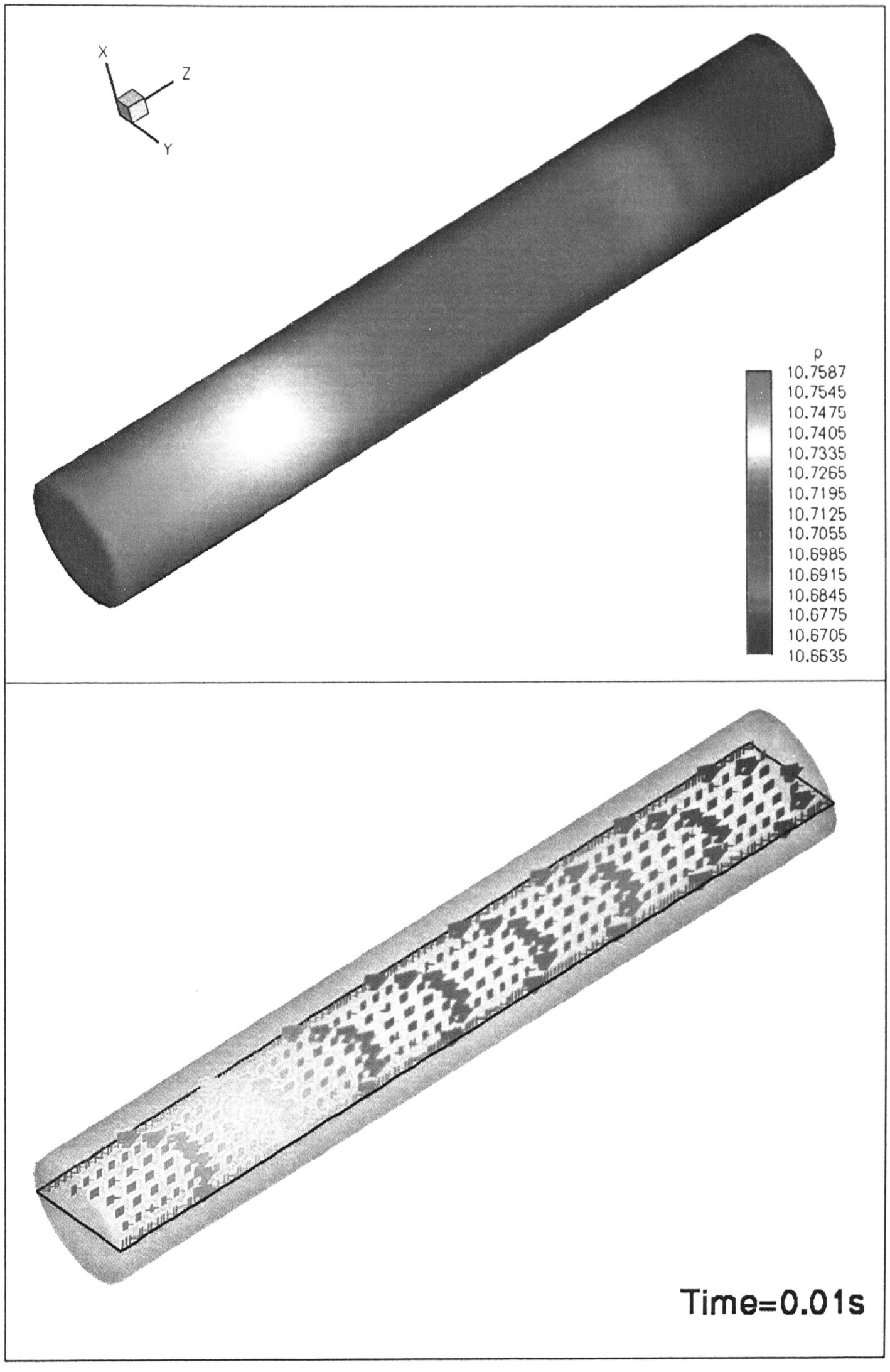


FIG. 6.1.2. Stokes problem

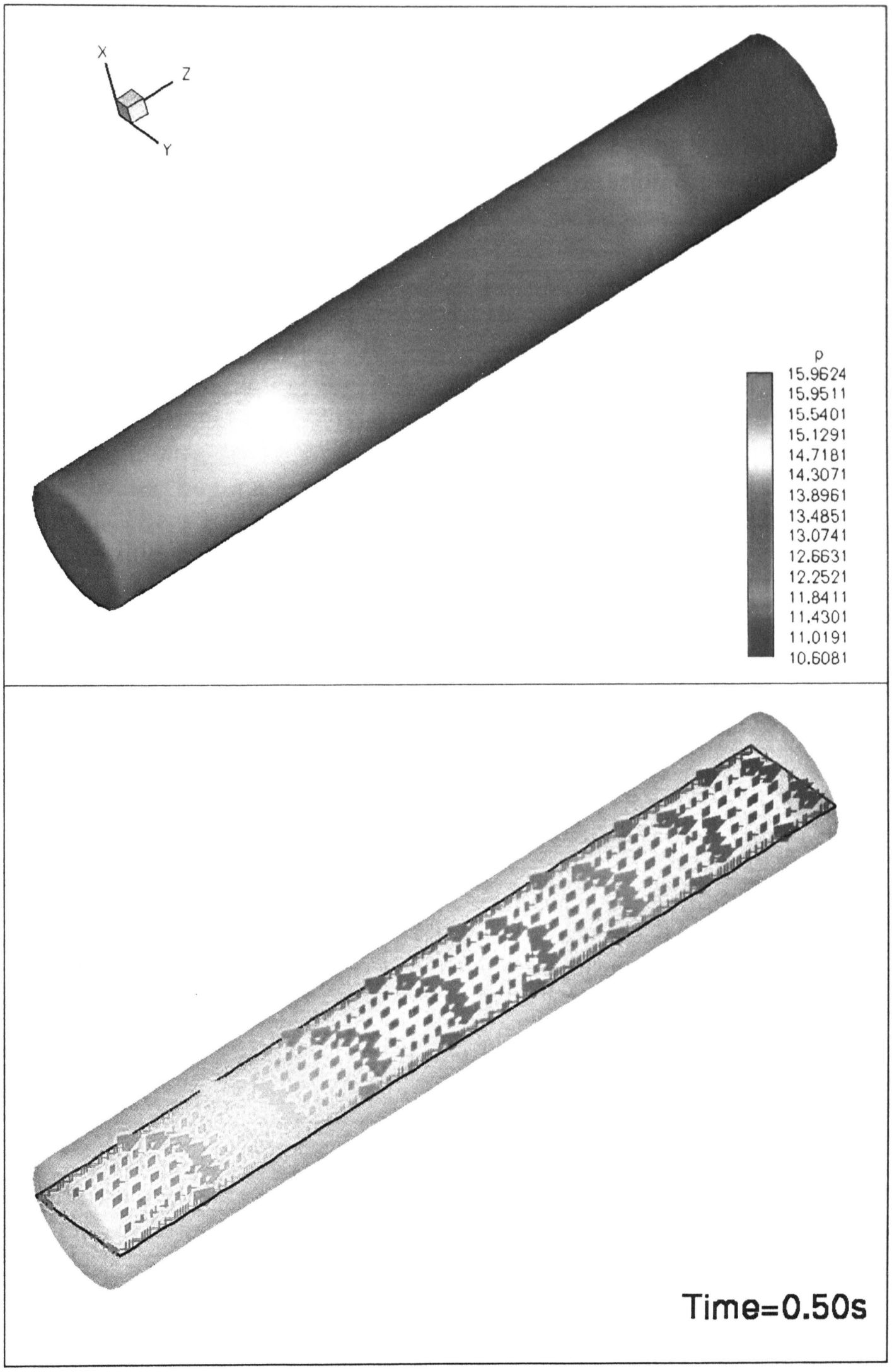


FIG. 6.1.3. Stokes problem

6.2 The Navier-Stokes Problem

The Stokes linear problem is a very bad approximation of the arterial flow. It is useful for the low Reynolds number, but by neglecting the convective term the possibility to model real geometry i.e. the flow past a solid profile is lost.

The model which includes the convective term is known as Navier-Stokes. In our formulation it suffices to omit the deformation ($\vec{u} \equiv \vec{0}$). The resulting nonlinear problem is very well solvable by the method which we have described earlier, till Reynolds number 1600. For higher Re we should use some type of stabilization, but for the arterial flow it is not necessary. The stabilization provided by the combination P2/P1 is sufficient for this problem.

For the verification of our method we have chosen the problem of flow past an isolated profile in free space (Fig. 6.2.4). The free space is simulated by the following trick. We prescribe nonhomogenous Dirichlet conditions on the outer boundary of the cuboid, in which the bypassed cylinder is inserted. There is a no-slip condition on the cylinder. The test proceeds in the following manner: it increases the fluid velocity on the cylinder surface up to the separation of a wake behind cylinder.

You can see Von Karmans vortex line on the presented results: as an animation on the CD in `/problem/ns2`, or as a picture, presenting the velocity field and pressure in sectorial view. The flow is constant with respect to the shift in the direction of the x axis. The result can be computed by the 2D computation as well.

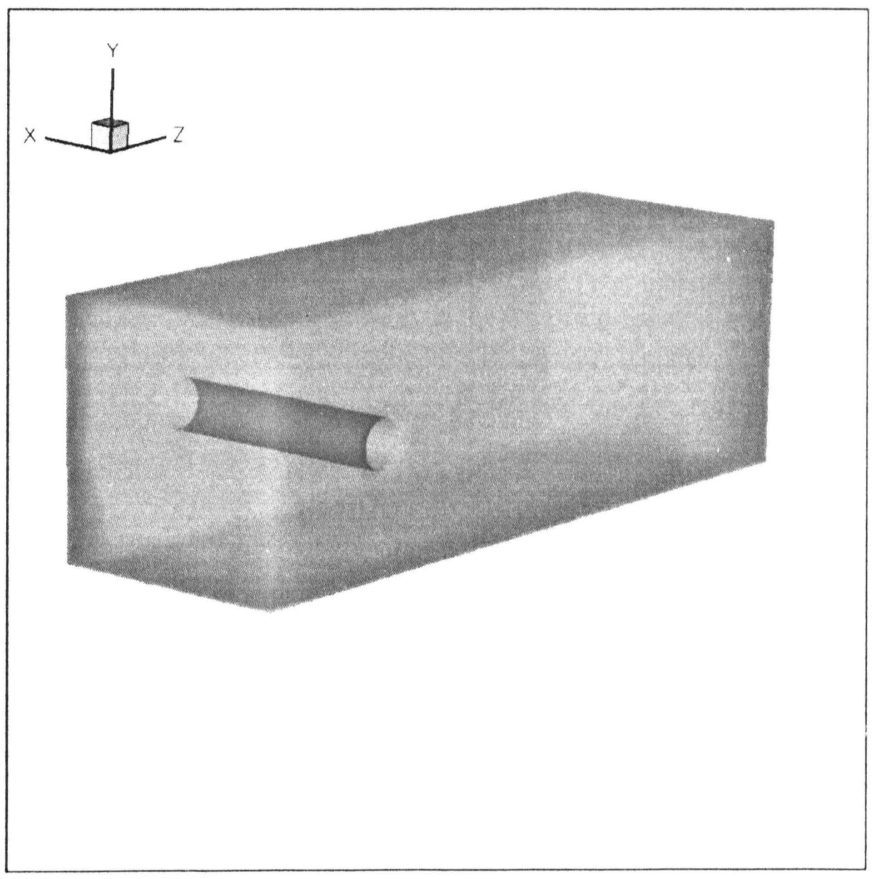


FIG. 6.2.4. Navier Stokes - test I

Vertices	7 517
Elements	40 442
Equations	177 272
Comp time	13 days
Time iters	458

TABLE 6.2.2.

An unstructured mesh is suitable for this problem. It allows a detailed description of the surface of the cylinder and its nearest environment. Simul-

taneously, by decreasing the number of elements in the direction towards the boundary, we were able to reduce the total number of elements. The constructed mesh (on Fig. 6.2.5) has 40442 elements, which corresponds to 177272 equations. The computation took 13 days.

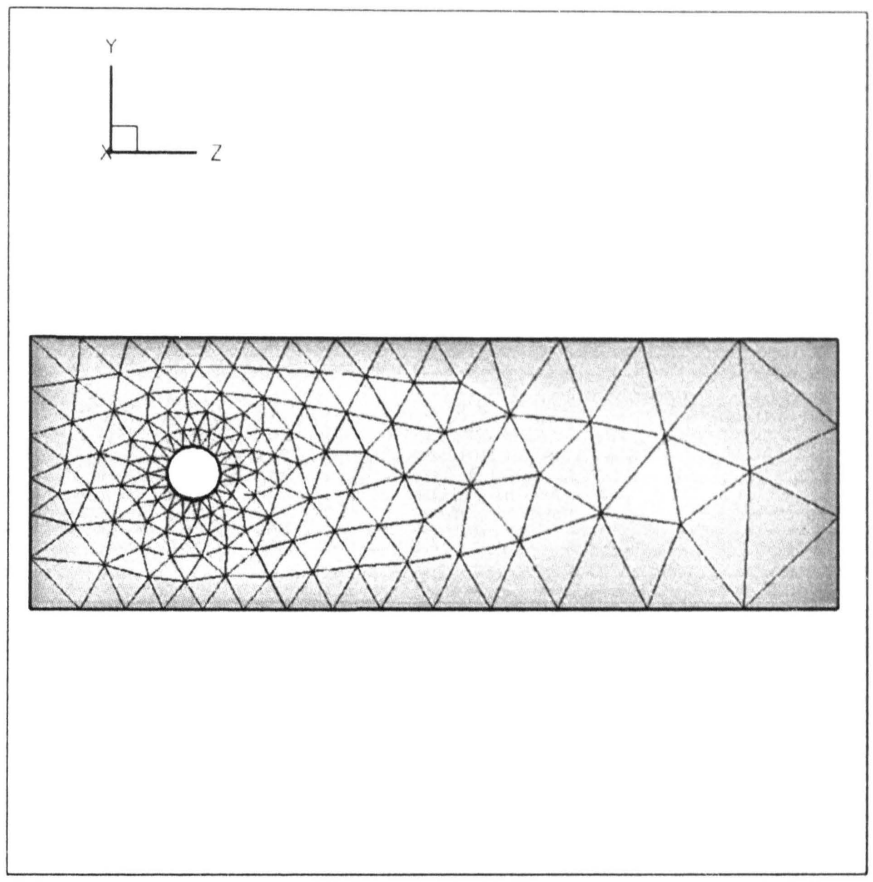


FIG. 6.2.5. Navier Stokes - test I - mesh

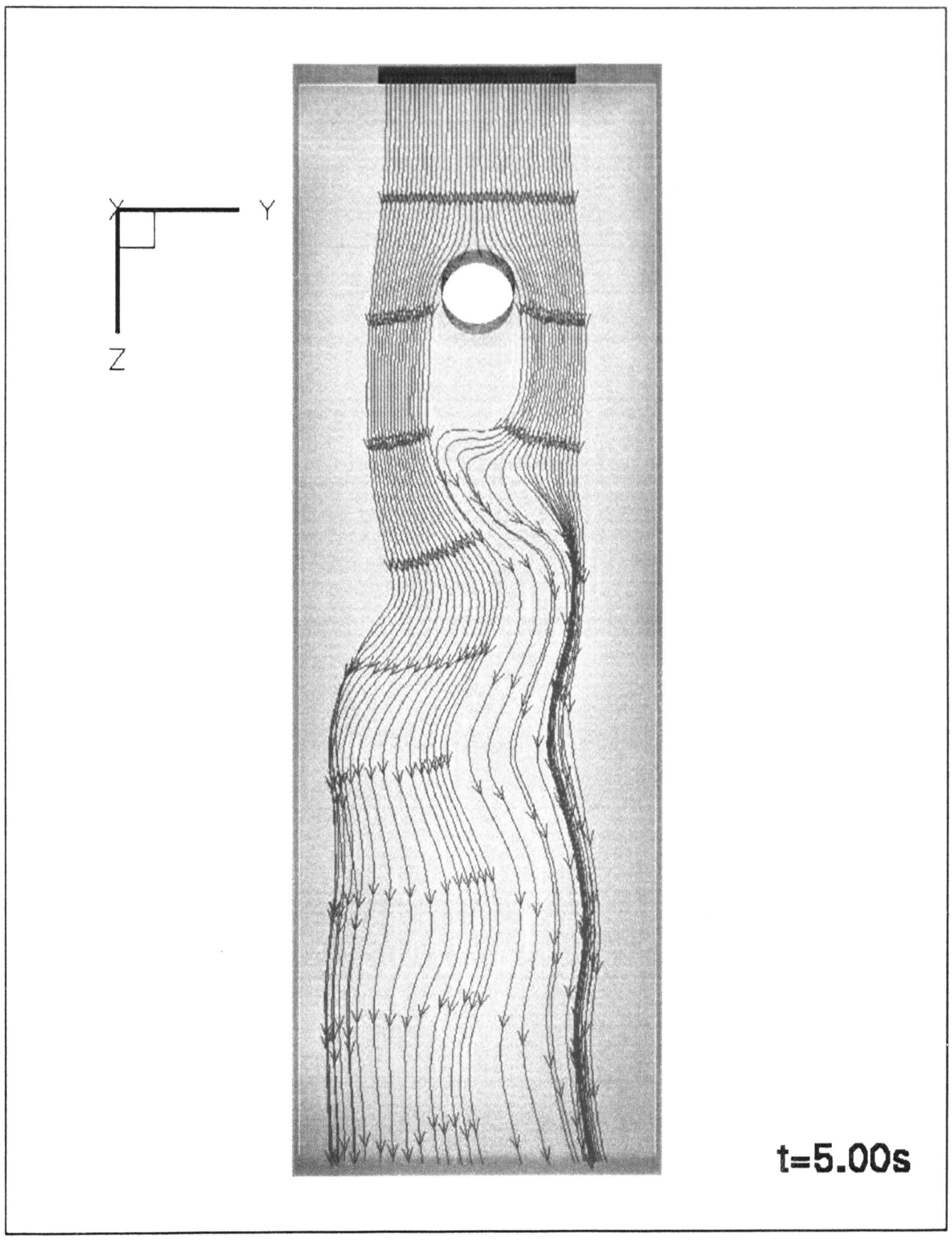


FIG. 6.2.6. Navier Stokes - test I

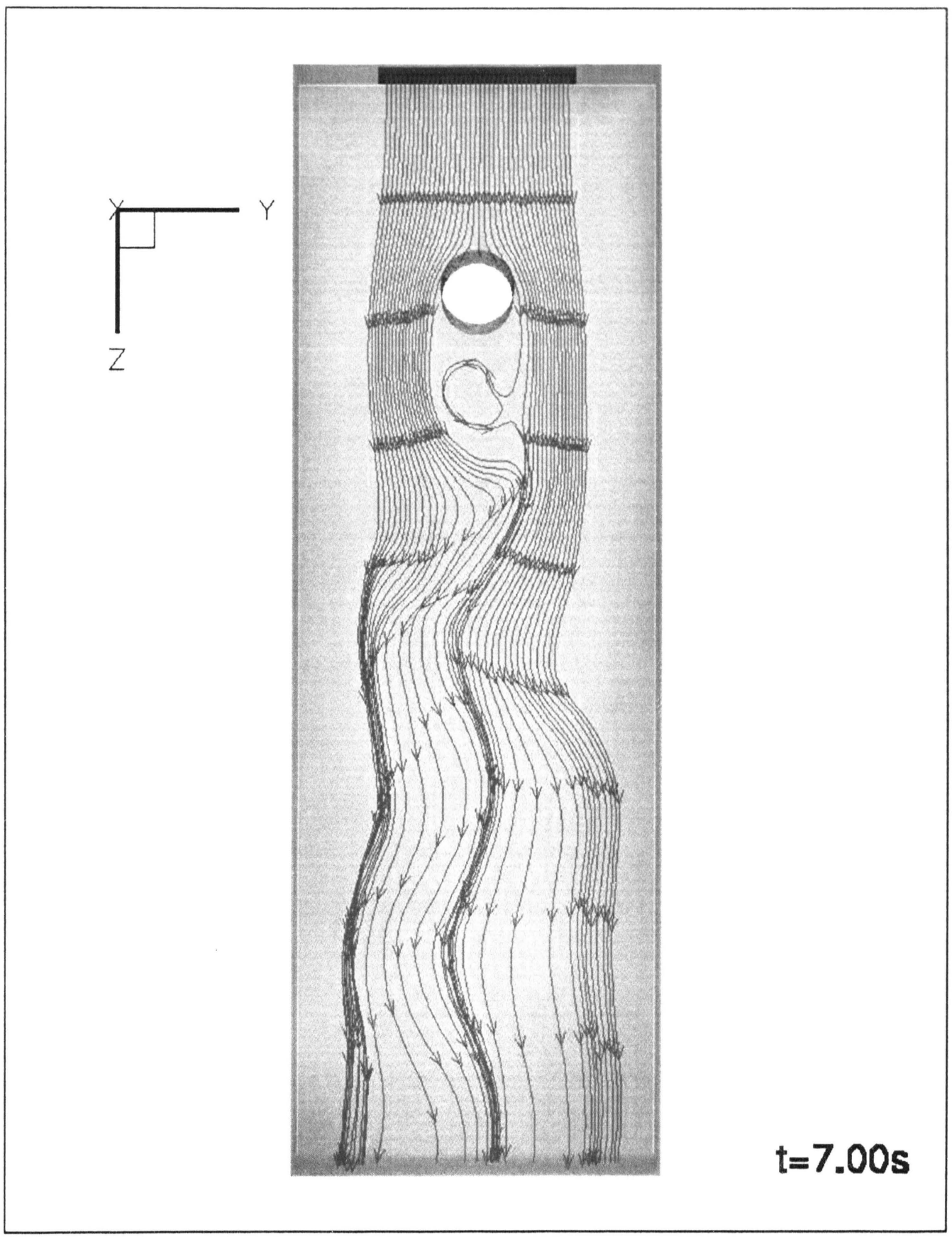


FIG. 6.2.7. Navier Stokes - test I

A more difficult problem for computation is the flow past a cylinder, which is closed into a tube (see Fig. 6.2.8). On the internal boundary of the tube there is the no-slip condition. This creates an effect, which is not present in the previous case: the interaction between the vortex flow behind the cylinder and the fluid on the tube boundary. As a test, the boundary conditions were chosen as follows: on the outlet there is free boundary, on the input there is a parabolical profile increasing with time. You can see the entrance of the vortex. The results are on the CD in `/problem/nsmalek`, but here we present only one frame with velocity field in sectorial view on the plane xz. This can be computed only by a real 3D computation.

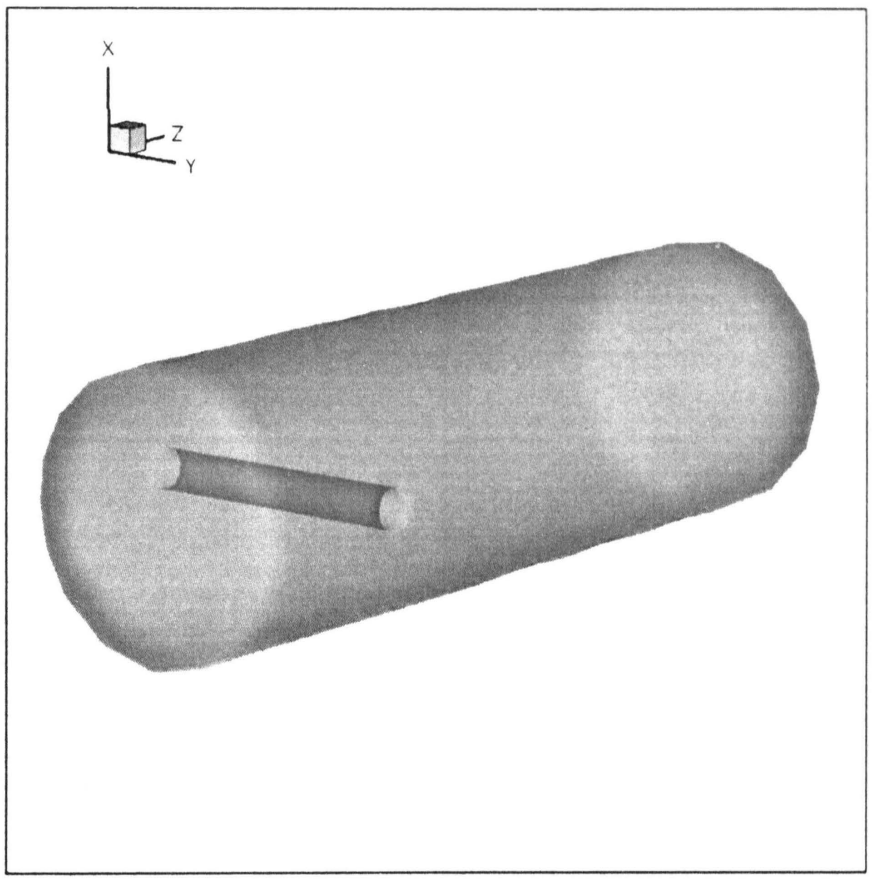


FIG. 6.2.8. Navier Stokes - test II

Vertices	4 107
Elements	21 316
Equations	95 044
Comp time	10 days
Time iters	422

TABLE 6.2.3.

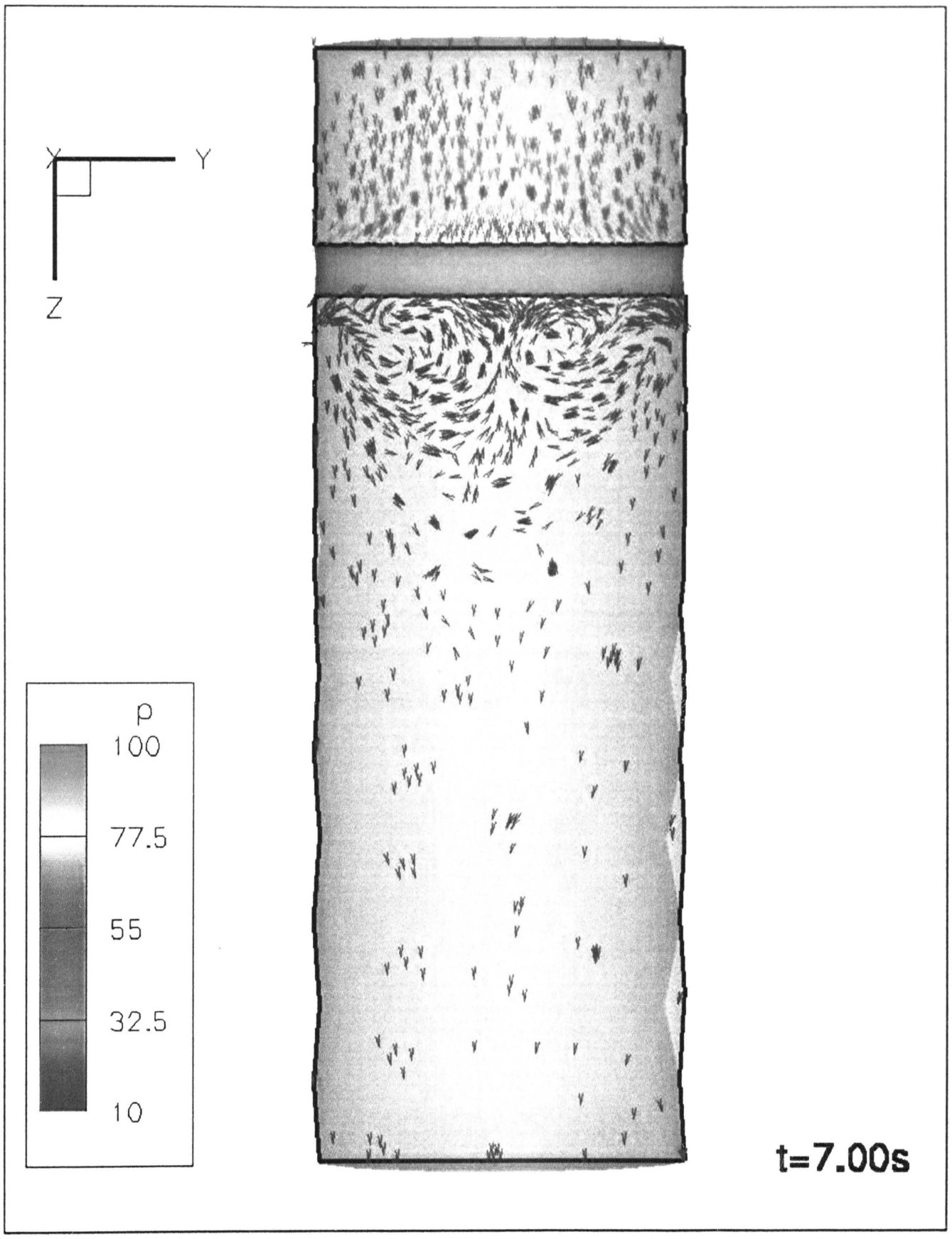


FIG. 6.2.9. Navier Stokes - test II

Y bifurcation (see Fig. 6.2.10) is a problem, which is very close to biology. It is the division of a vessel into two branches. The boundary condition corresponds to the flow driven by pressure gradient. Results can be found on the CD in `/problem/y3`. Here we present only one frame after 0.5 s of real time. At the picture there is the pressure and velocity field on the cut plane zy.

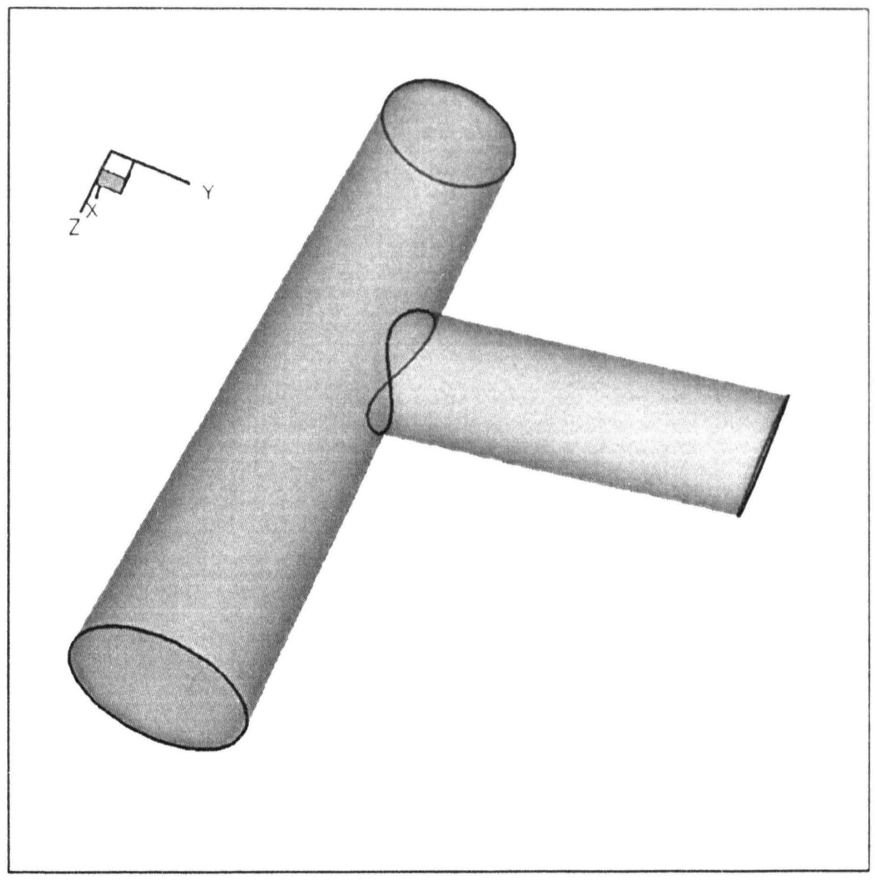


FIG. 6.2.10. Y bifurcation

Vertices	4 122
Elements	16 664
Equations	166 878
Comp time	2 days
Time iters	19

TABLE 6.2.4.

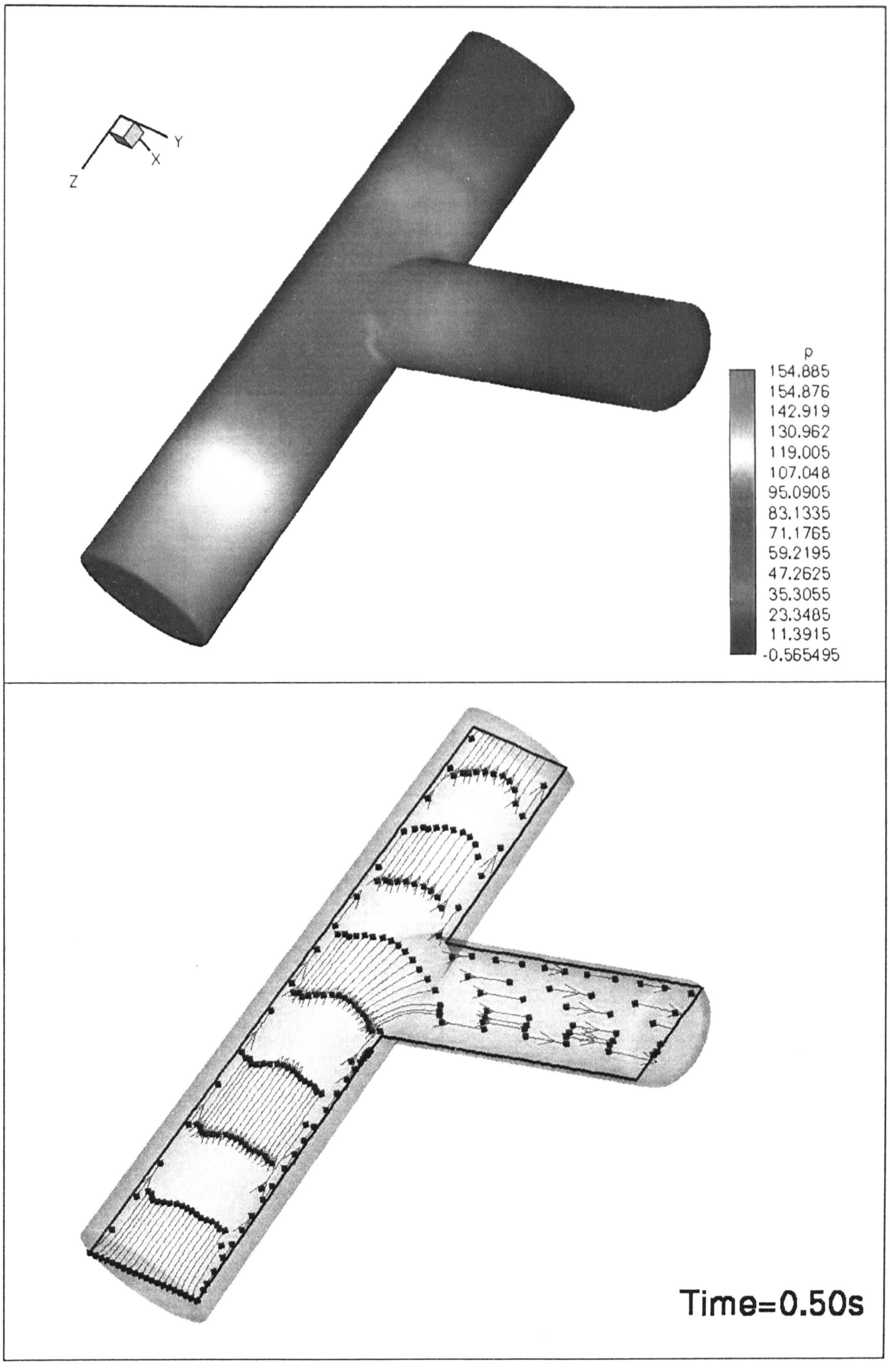


FIG. 6.2.11. Navier Stokes - test III

6.3 Elastic deformation

Our program can compute more than just flow. If we prepare a mesh which contains only solid elements, we can compute elastic deformation. We can see it on Fig 6.3.12. We stretch the bottom and the top of the object, and due to the incompressibility constrain we can see the reduction of the object diameter. At the following pictures we can see the initial and deformed state.

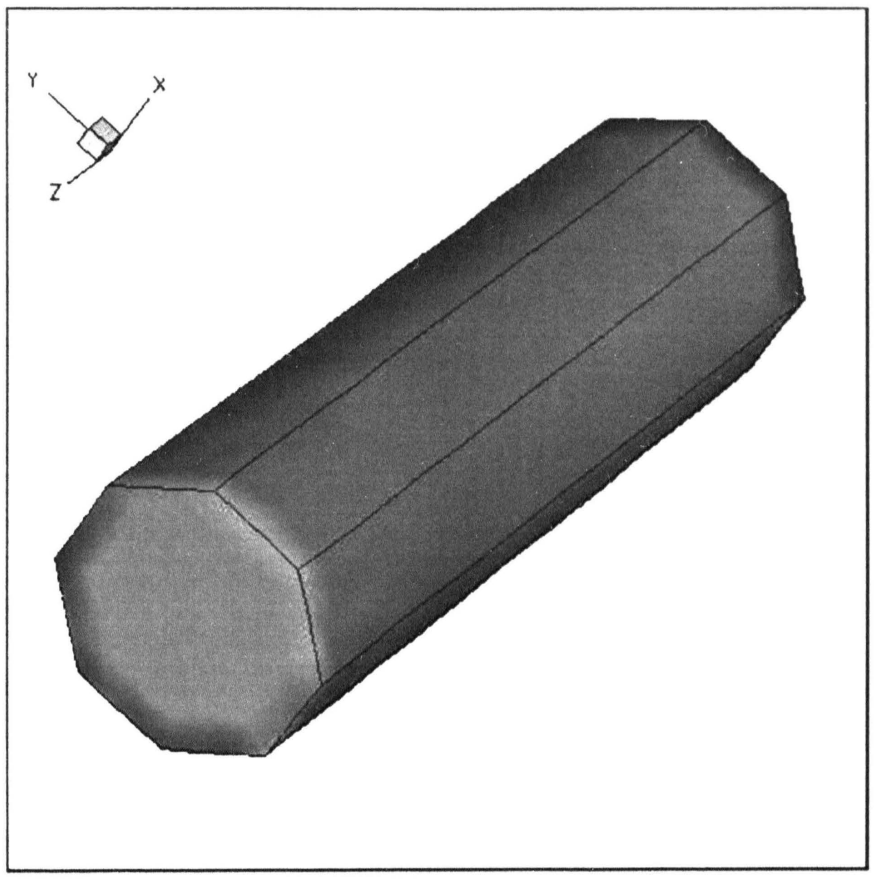


FIG. 6.3.12. Elastic deformation

Vertices	465
Elements	1 497
Equations	12 237
Comp time	12 hours
Time iters	63

TABLE 6.3.5.

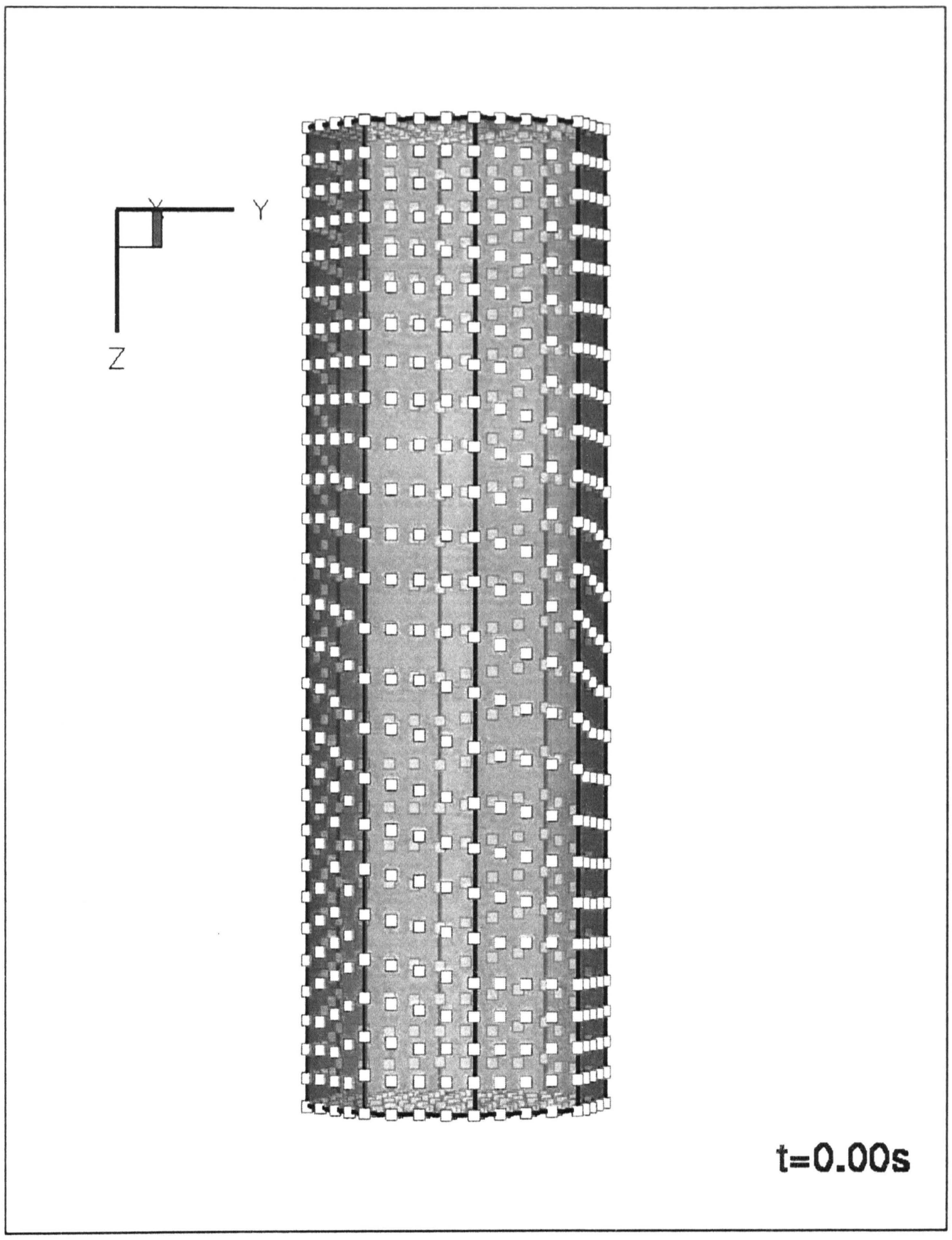


FIG. 6.3.13. Elastic deformation - Initial state

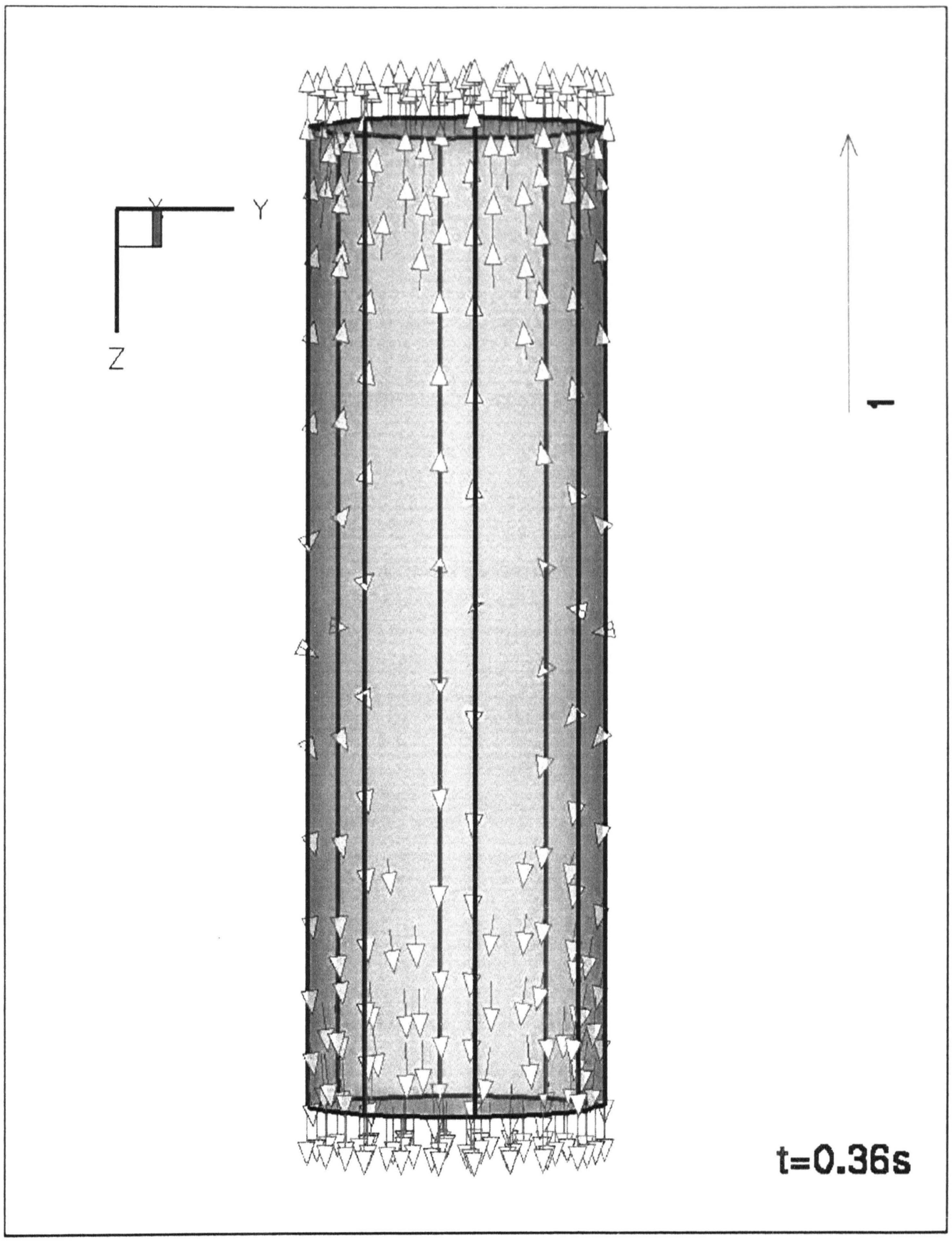


FIG. 6.3.14. Elastic deformation - Displacement in deformed state

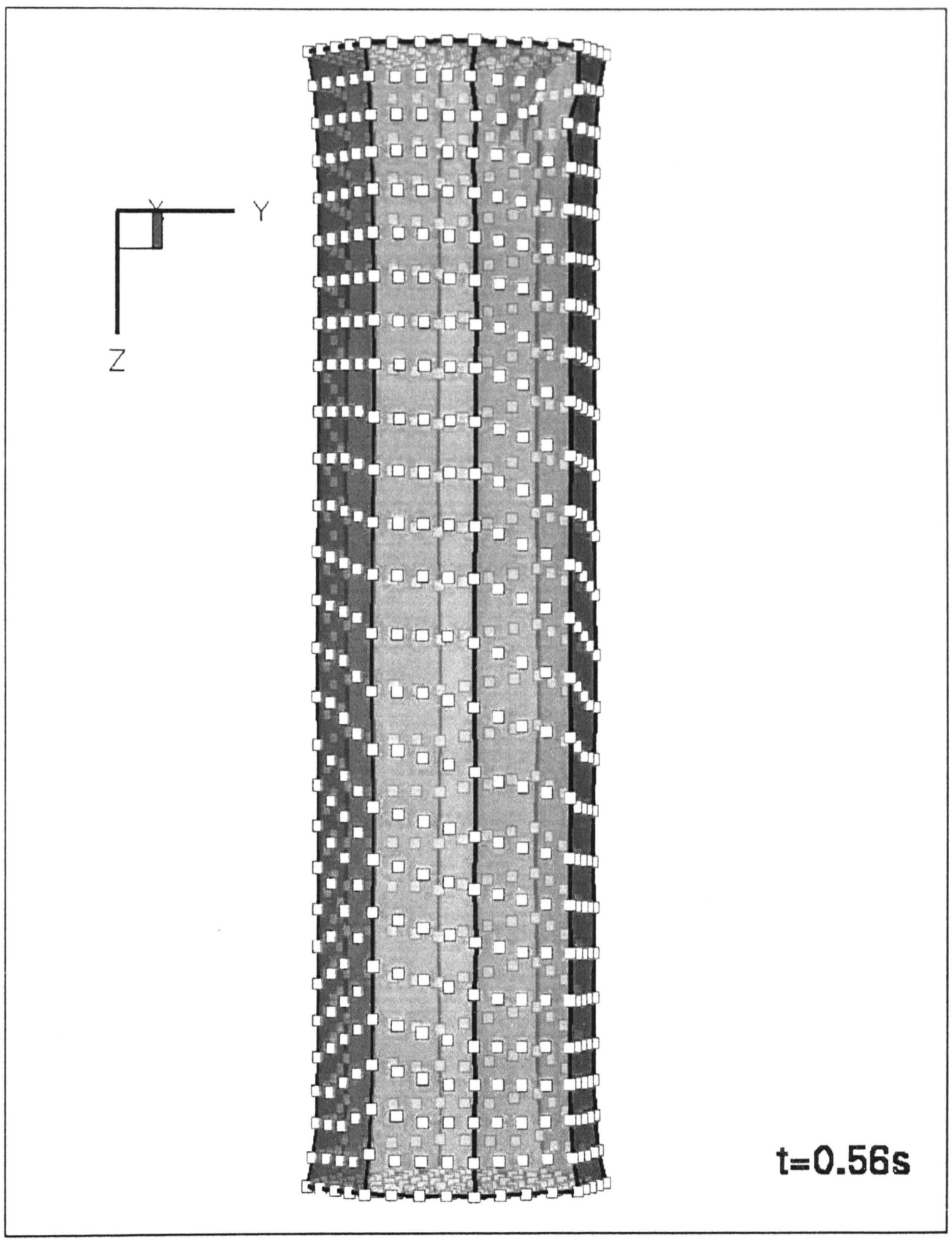


FIG. 6.3.15. Elastic deformation - Deformed state

6.4 Fluid-Structure interaction

The main aim of our approach is to compute the Fluid-Structure interaction. We must declare that not all problems which we started to compute were successfully computed. There are practicaly no analytical results, and our numerical simulations for low values of β resulted in non-physical behaviour.

The first problem is deflating a breathalyzer. The geometry is at Fig. 6.4.16. It represents a rubber breathalyzer filled with fluid. We prescribe the velocity flowing out of the ball and after some time we can see the volume of the breathalyzer decreasing. There is also an animation on the CD in the directory `/problem/breath`. Here we present only three frames (each picture is divided into solid (top) and fluid (bottom) part). On the last frame 6.4.21 there is velocity field in the deformed state. It confirms our target to compute the velocity and deformation fields together.

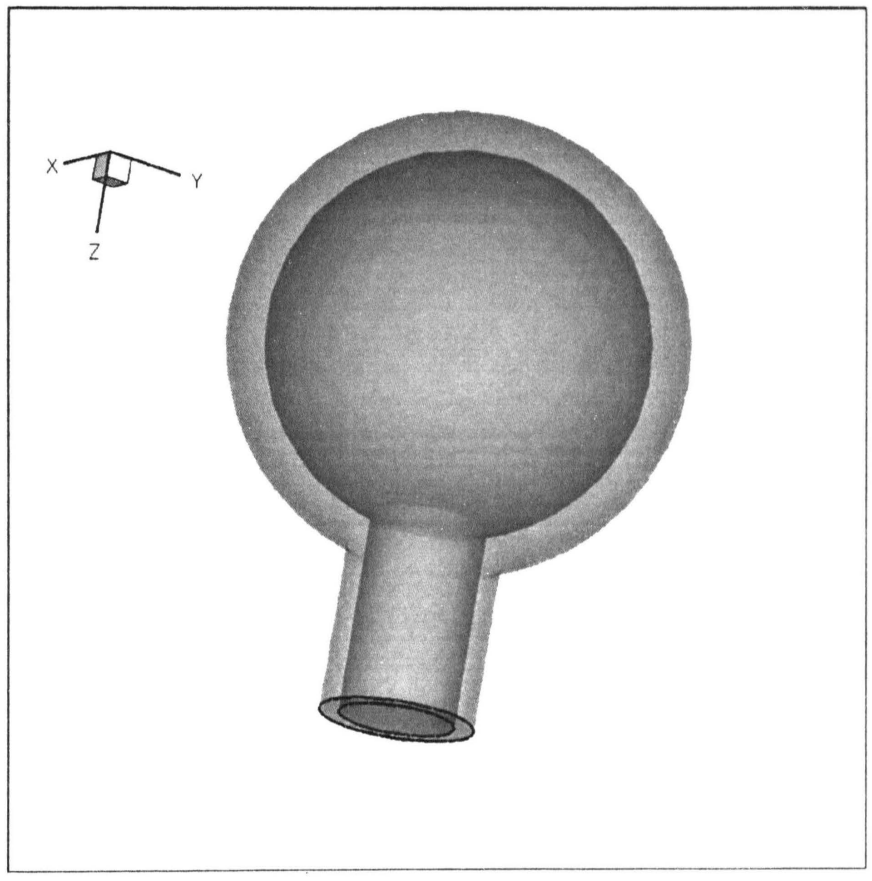


FIG. 6.4.16. Breath - Geometry

Vertices	1 389
Elements	6 508
Equations	48 771
Comp time	5 days
Time iters	1154

TABLE 6.4.6.

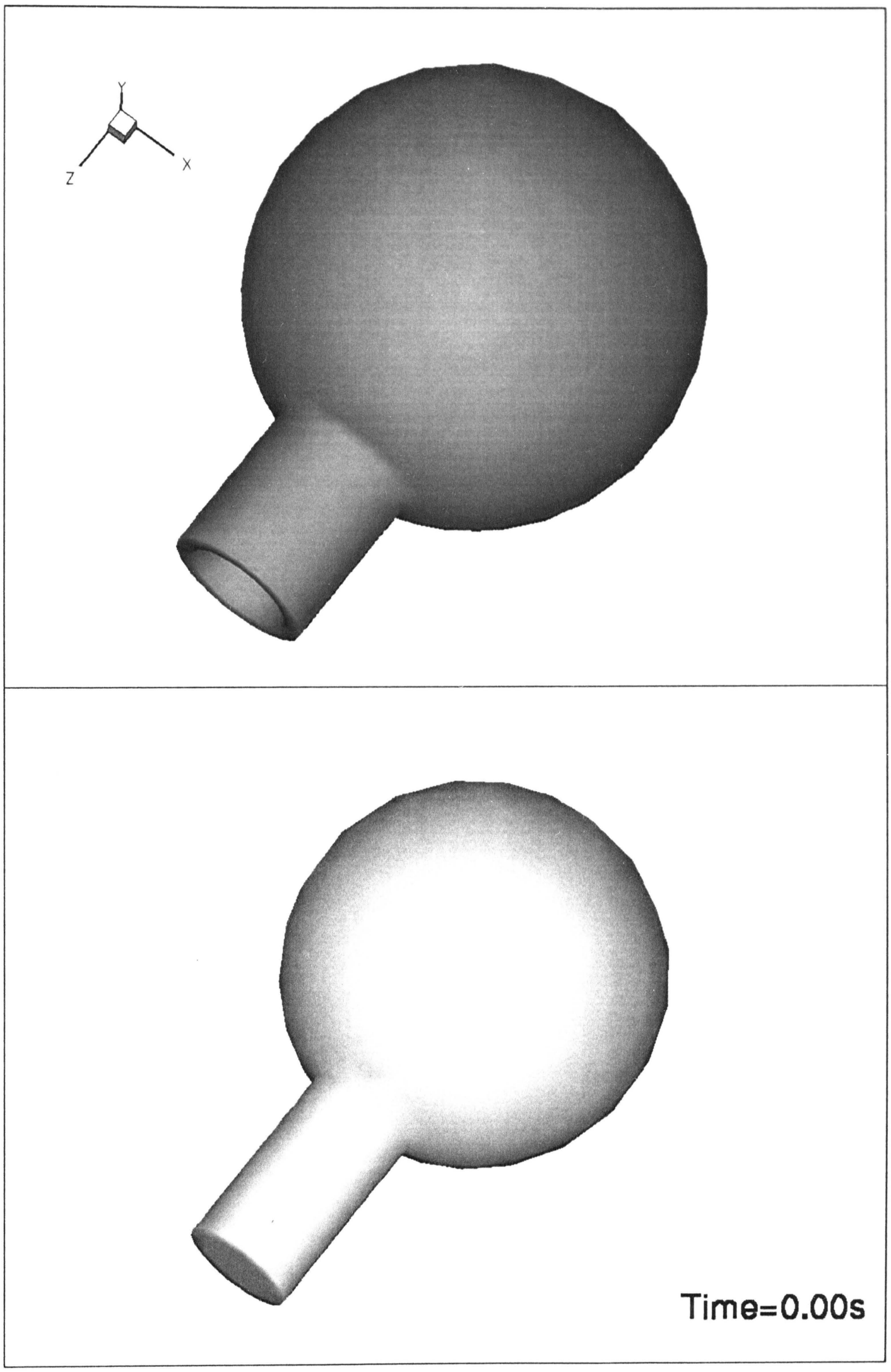


FIG. 6.4.17. Fluid-Structure interaction - Initial state

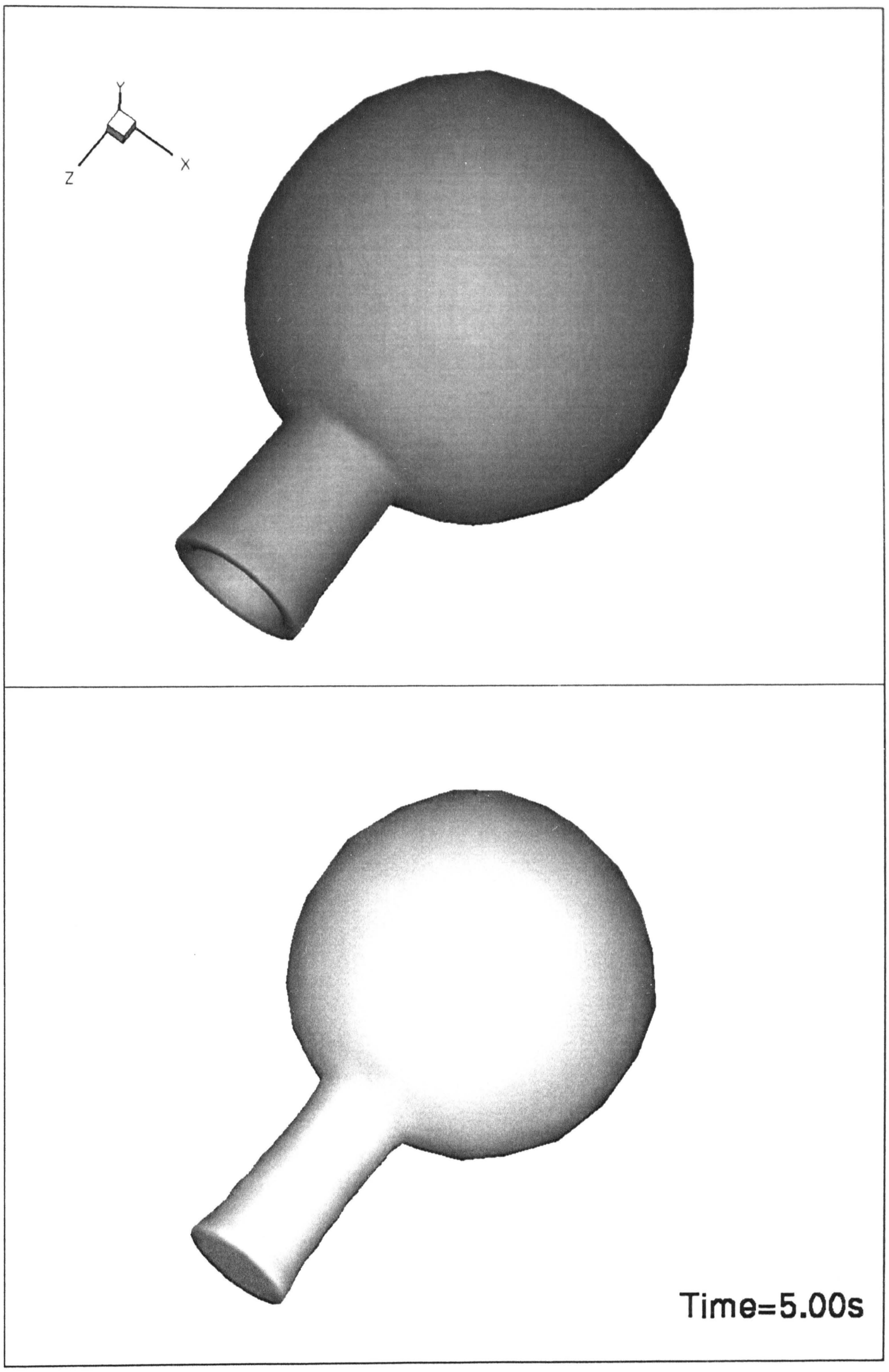


FIG. 6.4.18. Fluid-Structure interaction - Breathalyzer

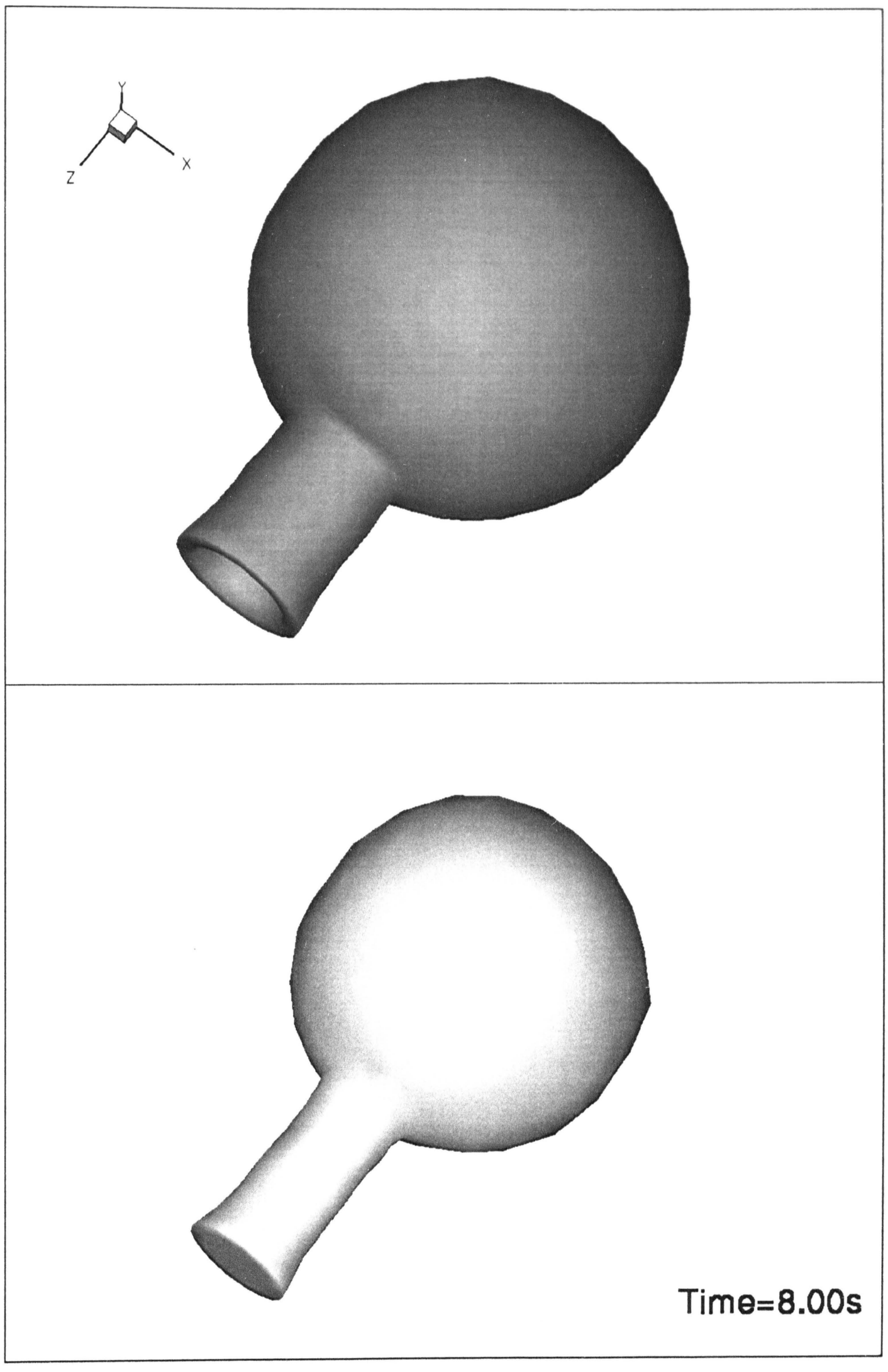


FIG. 6.4.19. Fluid-Structure interaction - Breathalyzer

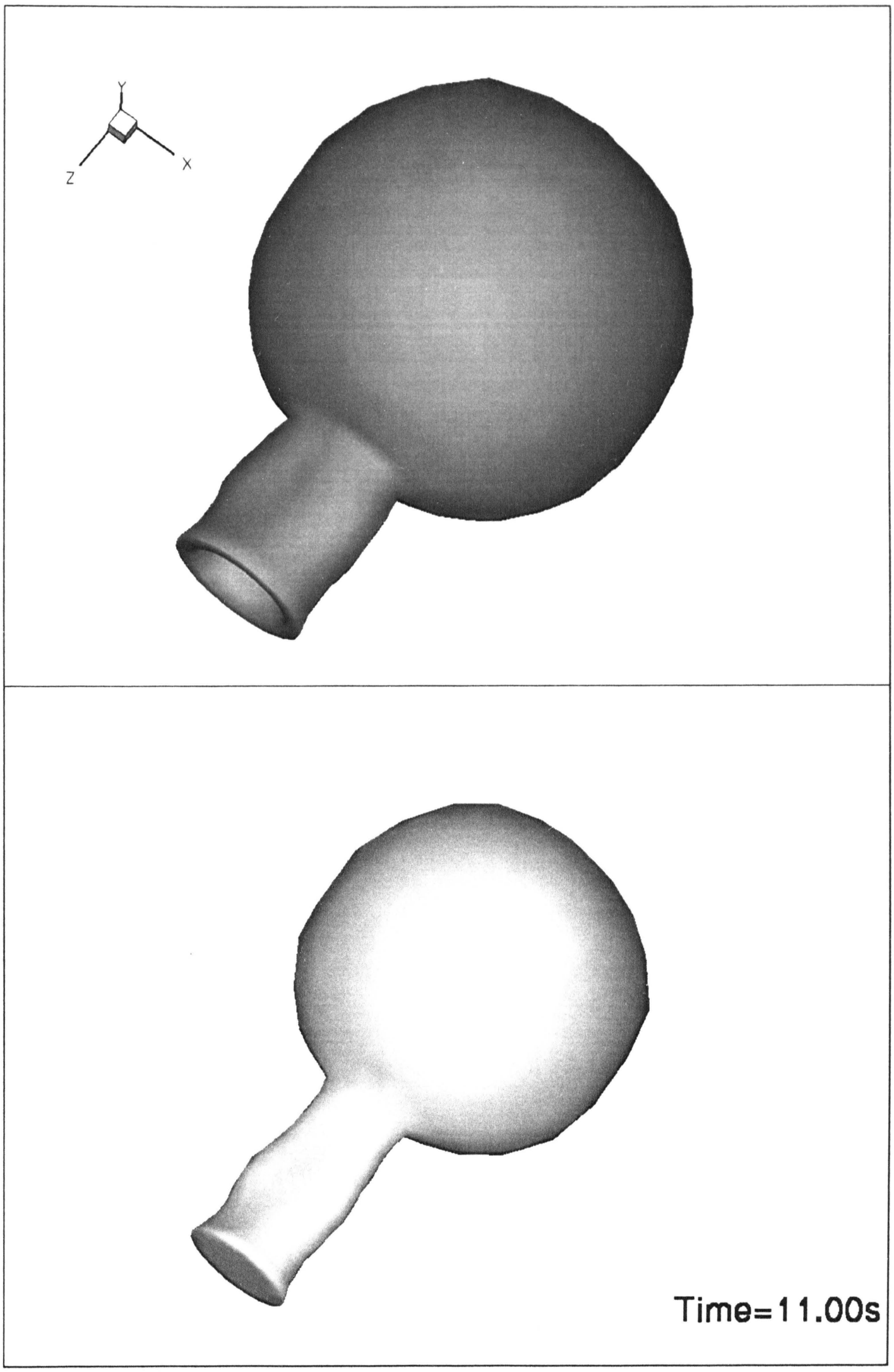


FIG. 6.4.20. Fluid-Structure interaction - Breathalyzer

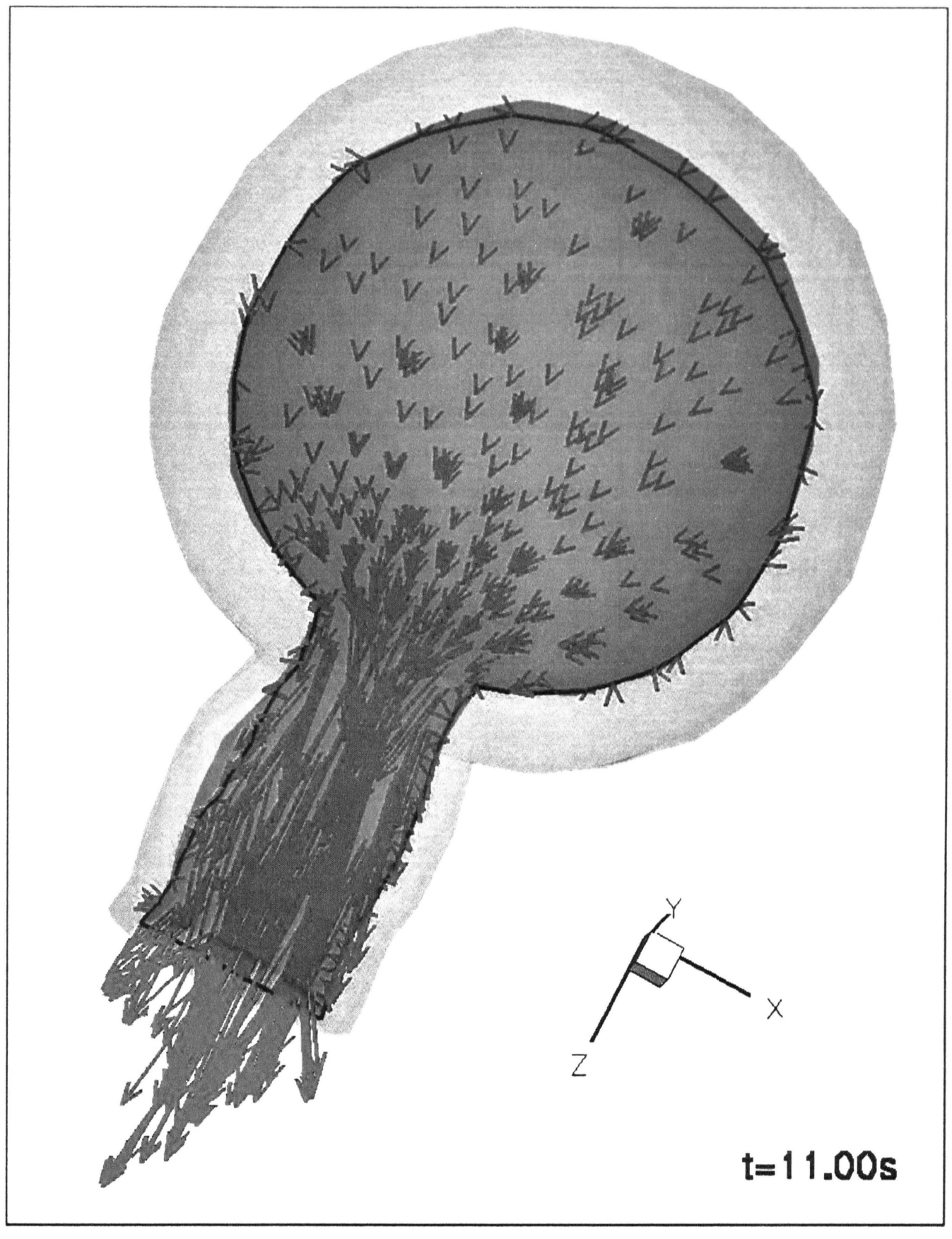


FIG. 6.4.21. Fluid-Structure interaction - Velocity in deformed state

The second F/S interaction problem is the flow past an elastic obstacle in a solid tube. The geometry of the problem is at Fig. 6.4.22. The obstacle is divided into two parts: non-elastic (closer to the boundary) and elastic. On the inlet we prescribe the velocity of flow into the tube and we can see the deflection of the elastic material in the direction of the velocity field. The whole animation can be found on the CD in the directory `/problem/obstfix`.

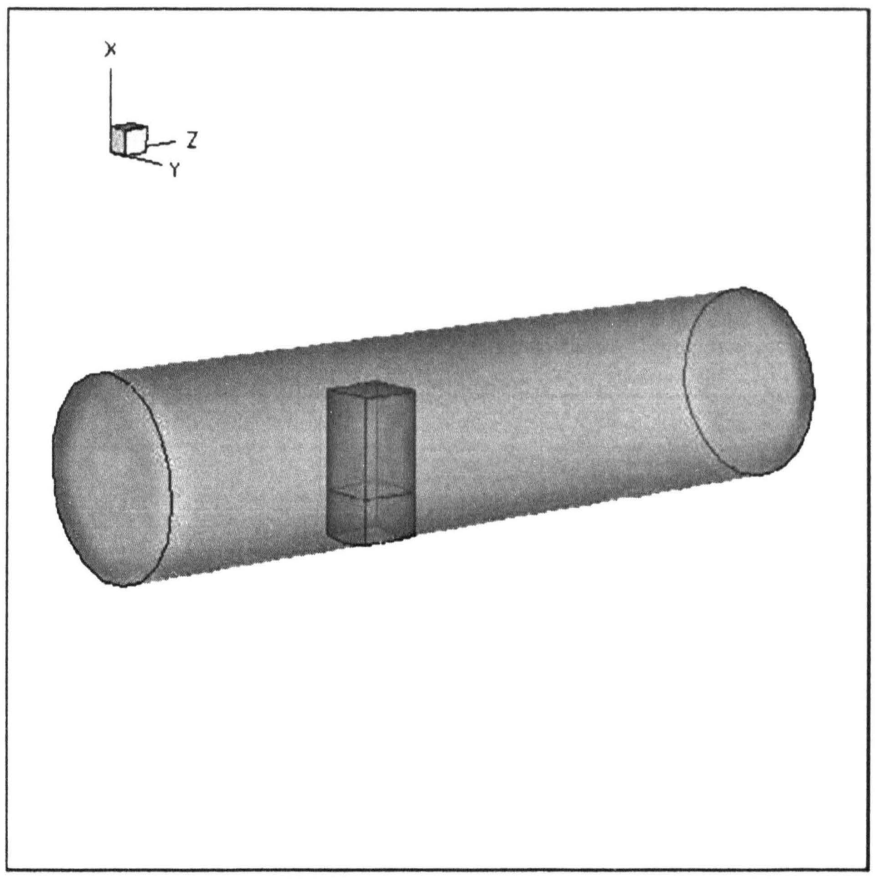


FIG. 6.4.22. Elastic obstacle - Geometry

Vertices	1 389
Elements	6 508
Equations	48 771
Comp time	16 hours
Time iters	37

TABLE 6.4.7.

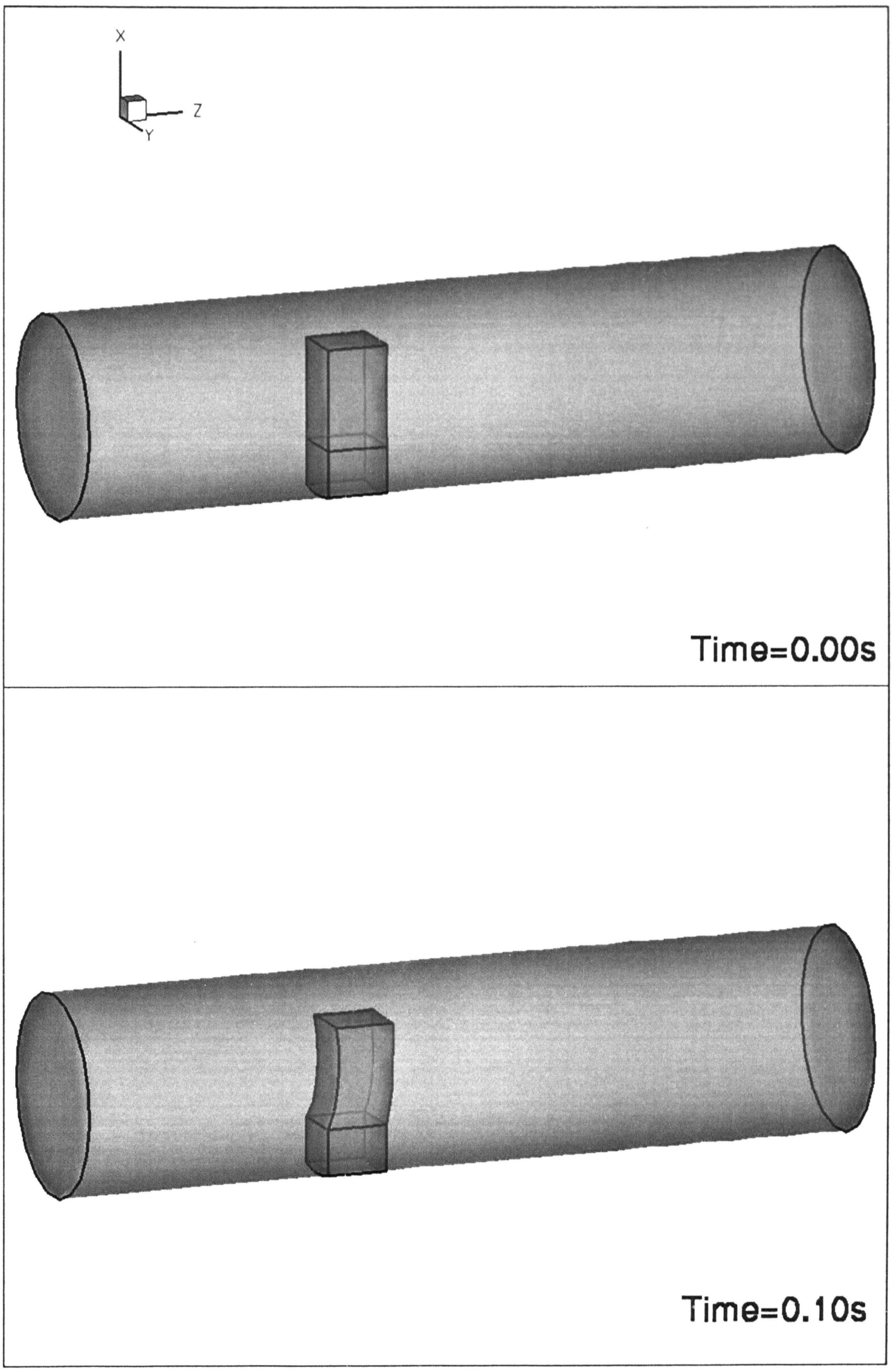


FIG. 6.4.23. Fluid-Structure interaction

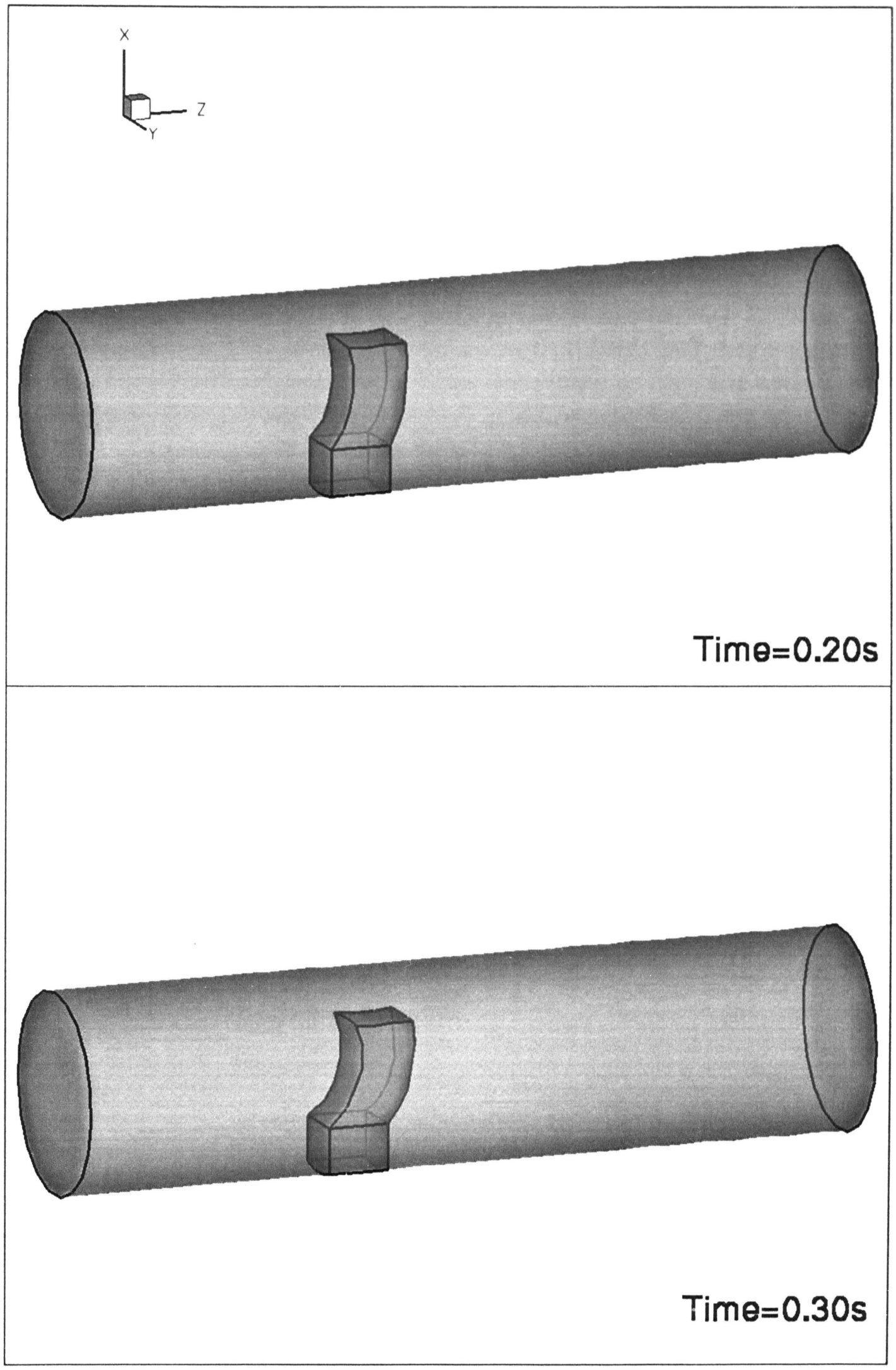


FIG. 6.4.24. Fluid-Structure interaction - Deformed state

CONCLUSIONS

In this work we have shown one of the possibilities, how to model the problem of flowing fluid surrounded by elastic solid material. We have tried to show the approach and method of derivation in this very new branch.

The main contribution of our work is our own program `FSTRIN`, which computes the solution of the time dependent problem in 3 space dimensions, using an unstructured mesh, which has the ability to describe even the most complicated geometries. The program is written in a general manner with the idea of extending it to more equations, which we hope to add into our model.

The directions, which we will try to extend our model to, can be divided into three branches:

1. Mechanical properties. The description of the artery wall was very simple. We would like to investigate the properties of more complicated solid materials. Also we will try to model the flow of blood in thinner arteries, which means using a different fluid model then the Newtonian one.

2. Physical / Chemical properties. As we state in the Anatomy chapter, remodelation is a very important property of living tissue. This phenomena has not been sufficiently described yet and we hope that we will bring some new results into this problem.

3. Mathematical properties. From the mathematical point of view we do not know anything about this model, even the question of the exstence ot the solution. This is big gap, which we hope to clear primarily.

BIBLIOGRAPHY

Brdička, M. (2000). *Mechanika kontinua.* Academia.

Hron, J. (2001). *Fluid structure interaction with application in biomechanics.* Ph. D. thesis, Charles University, Prague.

Humphrey, Jay D. (2002). *Cardiovascular Solid Mechanics.*

J. Valenta, B. Bo Šrámek, and František Klimeš (1995). *Biomechanics of the Caridovacular System.* ČVUT.

Joachim Schoberl, Hannes Gerstmayr, and Robert Gaisbauer (2003). Netgen - automatic mesh generator. http://www.hpfem.jku.at/netgen.

Lukšan, L. (2004). Numerické optimalizační metody. http://www.cs.cas.cz/ luksan/lekce4.ps.

Maršík, F. (1999). *Termodynamika kontinua.* Academia.

Satish Balay, Kris Buschelman, Wiliam D. Gropp, Dinesh Kaushik, Matt Kneplay, Lios Curfman McInnes, Barry F. Smith, and Hong Zhang (2001). Petsc home page. http://www.mcs.anl.gov/petsc.

Štembera, V. (2003). The flow through visco-elastic tubes. Master's thesis, Charles University, Prague.