

HIERARCHICAL MODELLING IN BIOLOGY: A SYSTEMATIC BUILD-UP OF A LIMB MODEL

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Abstract

A multi-level model, that provides a hierarchically structured description of a complex, multi-scale limb system is proposed in this report for predicting and analyzing movement patterns generated by various activation signals. The levels, the sub-models on each level and their interconnections are developed and described following a systematic modelling procedure.

The computational properties (degrees of freedom and differential index) of the developed model are analyzed and some of the sub-models are transformed to meet the index-one requirement for solving the resulting differential algebraic equation (DAE) model.

A solution method is implemented in MATLAB that is able to simulate the dynamic movements of the limb (movement patterns) given the variations of the activation signal in time as the model input. The model is extensively verified against engineering expectations by using parameter values found in the literature, and a good agreement was found.

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Chapter 1

Introduction

1.1 Aim and related results

Limb modelling Human locomotion is a complex movement of a body. For a successful movement, interactions among muscular-skeletal system and central nervous system (CNS) are needed. The CNS controls the movement by sending activation signals to the correct skeletal muscle at correct moment. The effect of this signal is that the muscle initiates a movement by exerting force to a body segment. Even in the case of a simple movement the contribution of a large number of muscles of different size and shape is necessary. A common movement such as locomotion require more muscles. With a feedback system that uses different kind of receptors, the CNS controls the movement. In healthy humans all these complex coordinated actions lead unconsciously to a smooth movement.

However, in the case of disease or accident an impairment causes that this interaction is out of order and this affects the ability to move smoothly or to move at all. For the development of techniques and/or systems to restore control and reduce disabilities, detailed knowledge is needed about the muscle-skeletal system and CNS. We have to know how the muscle exert force, what factors effect this force, how does the movement pattern depend on the muscle force, how does CNS sense the state of muscle, etc. Examining motions using models help us to find out more about muscles and movement pattern generation.

The models of dynamics of human musculoskeletal system contains the equations of multi-rigid-body system and the equations of the dynamics of muscle contraction. The crucial component of this system is the model that generates the exerting muscle forces.

To create a realistic model of limb a lot of different effects must be taken into account. It means that there are a lot of processes that have to be modelled, such as chemical reaction, biochemical processes, material and structural properties of the muscles, etc. A common used model only deals with one or at least some of them, so if we would like to model the most of these processes then we have to connect some models and we have to create an interface among them.

Muscle modelling: Different muscle models exist that focus one or more important aspects of muscle functioning. Some of them deal with individual muscle characteristics and some of them deal with generalized muscle characteristics that are valid for all muscle. But most of the existing models deal only with a partial functioning of the muscle such as a force depending on the muscle length or muscle geometry or firing rates of nerves etc. The most important model types are as follows [40]:

- *Hill-type models:* were created by Hill [17] based on experimental observations. This model consists of serially arranged contractile elements connected with springs. The contractile element represent the contraction machinery while the springs represent the contribution of tendon and aponeurosis. This model contains a third type of elements that are arranged in parallel with the first two elements. This third type element represent the passive muscle properties. This model was modified by some authors, e.g Hatze [15], to increase the capabilities of predicting force of different muscles. A Hill-type model describes the interaction of contractile machinery and the series of elastic structures. This model is generally used when the movement of the limb is simulated e.g. by Lim [30] for e.g. examining the muscle properties in different circumstances like Garrison [12] or examining another muscle model like

Ettema [10] and Bogert [39], or when the control strategies of the movement are tested like Karniel [22] and Myers [33].

- *Cross-bridge models*: were proposed by Huxley [21] based on by cross bridge dynamics. Using this model, the force-velocity characteristic and the energy metabolism can be described and the exerted force of muscle can be investigated in time. This model was extended by some authors, such as Cole [4], Derényi [5], Duke [6], Eisenberg [7] Hill [18], Ma and Zahalak [31], Wu [43], and was approximated by e.g. Zahalak [45] to model the force transients, energy utilization and excitation dynamics in more detail.
- *Morphological models*: are based on the fact that the exerted forces are strongly related by morphology. It means that these models combine the geometrical properties of muscle and tendon e.g., their length, angle between fiber and aponeurosis. The basis of these models is that the muscle volume is constant during contraction. This model has been realized in both 2D [20] and 3D [42]. These models try to predict the muscle geometry and the isometric force-length curve. By developing these models e.g. Otten [34] and van Leeuwen [29] modelled the uni- and bi-pennate muscles and they predicted the mechanically stable muscle geometries.
- *Morpho-mechanical models*: are based on the finite element method (FEM). Such models are developed for cardiac muscles, smooth muscles and skeletal muscles [40]. This method takes into account all specific structural and material properties of the skeletal muscles including those that have been mentioned earlier in other type of limb's model. These models assume that the muscle tissue is a continuum. This makes it possible to study the mechanism of force exertion of muscles in more detail.

There are same models that deal with the movement pattern generation according to the force exertion and neuronal input. For example Cheng et al. [3] create this kind of model, but they model only the force exertion and they do not deal with sarcomere. The movement pattern is generated by an existing skeleton dynamics program. Lim et al. [30] also create a model of movement generation from the neuronal input, but they do not deal with sarcomeres and fibers. They use the Hill's muscle model. There are a lot of models of movement generation based on the force exertion, but most of them are deal with only a limb containing two or three joints and usually same (one extensor, one flexor and sometimes one or two pieces of two-joints muscles) muscles at each joints. For example Yakovenko et al [44] examined the contribution of stretch reflexes to locomotor control using a model containing two pieces of three-joint legs. Gunter and Ruder [13] tested the λ -model using model containing two pieces of three-joint legs and fourteen muscles per leg. Myers and Massone [33] investigated the robustness of plant properties in point-to-point arm movements using a two-joints model with six pieces of linearized Hill's muscles. Karniel and Inbar [22] investigated the motor learning of human reaching movements using a two-joints model with six pieces of Hill's muscles. In case of these models the inputs of them were the neuronal activation.

Hungarian scientific background and the roots of the limb model: Modelling of limb movement patterns based on neuronal activity has been developed in Hungary for some years. Differential neuro-muscular-skeletal structures have been studied by Laczko et al. [26, 25, 24] using mathematical models and computer simulation. Tihanyi and Lackzo developed a computer simulation to analyze the effect of motor unit recruitment pattern and muscle fiber distribution on whole muscle force generation [38]. Lackzo et al. also proposed to study the link between neuronal, muscular and skeletal systems using a mathematical model that simulates muscle contraction and that resulting joint rotations as a function of motoneuron activity. They proposed and developed a concept to model the effect of neural and biomechanical parameters and properties of limb movements on movement patterns that are generated. In Hungary, the principal investigator of the OTKA grant titled "Control of movements of multi-joint limbs - an electro-mechanical model" developed the ideas for modelling joint rotations and limb movements as a function of motoneuron firing frequencies. This is an ongoing work supervised by Laczko in the Research Institute of Technical Physics and Material Sciences and at the Faculty of Physical Education and Sport Sciences of the Semmelweis University in strong cooperation with the New York University School of Medicine. Their general, complex limb model takes into account geometric and inertial properties of the limb, the muscle force-length and force-frequency relationships, passive forces, gravitational forces, maximal isometric forces, muscle attachment points and force-(contraction)velocity relations, and a load parameter that simulates the effect of body weight. They study the sensitivity of movement patterns to these parameters. The simulation of rat hindlimb movement

during swimming has been developed as an application of their models [27]. An enhanced version of that model is being extended with muscle force-velocity relationship and is being applied for rat walking [28]. The biomechanical and neuro-mechanical aspects of the limb model described in the present report originates from the above mentioned grant and studies and uses a multi-scale programming method that has been successfully applied in other scientific fields.

To summarize the properties of the existing models in the literature, we can say, that they usually only focus on a certain aspect or mechanism and/or contains two or three joints and some muscles without any attempt to describe a human movement in a global holistic way.

Hierarchical (multi-scale) modelling Most of complex biological and medical systems are inherently multi-scale systems. The reason for this is, that the modelling of these systems has its roots in physics, chemistry, biology and bio-physics, thus the properties of models reflect the underlying time and length scales on which important phenomena occur. This can be from the quantum mechanical length scales of 10-13 nm with time scales of 10-16 ns to global scales of 1 m and 1 s and higher. Besides of biological and medical systems that are of interest here, many theoretically interesting and practically important other systems, for example process systems, systems in nuclear physics, ecology etc. also exhibit multi-scale nature.

Despite of the above, there is no matured way of constructing multi-scale models, that is why much research effort is concentrated to this area. Several papers deal with the development of various multi-scale process models (see e.g. [2, 14, 35]) from where a methodology could perhaps be extracted. At the same time, results are also emerging in the field of integrating sub-models into a multi-scale process modelling framework [2].

Aim Therefore, our aim is to create a general framework of modelling that is able to describe the movement pattern based on the neuronal activation, molecular events, and muscle force exertion. To realize our aim, different kind of partial models have to be integrated because these partial models deal only with one or some aspects of force generation. In order to integrate them, these various aspects should be handled and the interaction of these aspects should be modelled, too. It means that a complex model will be created. The granularity of description should be tunable according to the requirements. Of course, the validation of model must be done based on measurements. It means that the final model won't be very detailed since the parameters must be estimated.

Analysis of model should also be completed. This analysis means the solvability analysis of the model using numerical methods, the sensitivity analysis of the parameters, parameter estimation, etc.

In order to demonstrate the capabilities of our general framework a simple case study is used that integrates the following models known from the literature:

- model of recruitment of motor units: [3].
- model of sarcomere: [5]
- model of active force generation (force-length, force-frequency relationships) such as [3, 9, 11, 19, 27, 28, 40, 44]
- model of passive force: [4] that is similar to the [11, 27, 28, 44].
- model of elastic properties of tendon: [3, 9].
- model of aponeurosis and pennate effect: [40, 41].
- model of limb dynamics: a well-known limb dynamic equations are used: [8, 47]

1.2 Modelling problem statement

1.2.1 The limb system

A limb system contains two main elements: the segments (bones) and muscles. Segments give the solid frame of the system while the muscles with tendons and aponeurosis determine the dynamics of the limb.

Muscles exert force and these forces effect the joints and segments via tendon and aponeurosis and rotate the segments. The basic force generation element is the sarcomere where the two contractile filament, the actin and myosin, produce force during they slide on each other. We call this mechanism the cross-bridge mechanism and sliding filament theory.

There are more serial and parallel connected sarcomeres in the fiber. The fiber integrate the forces of sarcomeres. The fibers are organized in motor unit. Motor unit contains similar fibers and these fibers are excited by one neuron. The number of fibers in a motor unit depends on the motor unit. If it contains few fibers than this motor unit can be controlled more precisely. A muscle contains different kind of motor units that are connected in parallel. There are tendons and/or aponeuroses in both ends of a muscle. They have got viscoelastic properties and they transport the exerted force to the segment. Each part of the muscle have got intrinsic, passive properties influencing the exerted force.

The line of pull and the line of fiber are usually not arranged in parallel way. In this case we say that the muscle is a pennate muscle. Pennation effects the force that the tendon senses.

Our limb model mainly concentrates into the mechanical properties of the muscle and limb and not deals with very much to the electrical properties of the muscle. It means that the muscle force depends on several factors while the electrical activity of the muscle does not model. The most important factors that influences the muscle force are:

- length of the muscle
- current velocity of the muscle
- firing rates of exciting nerve or activation signal
- passive, mechanical properties of muscle tissue
- geometry of the parts of the muscle
- viscoelasticity of the tendon and aponeurosis
- interaction among the parts of muscle.

If one wants to construct a complex, detailed model these effects should be modelled. Since our model will contain more parts the information transformation among them must be well defined. There are variables of the muscle that represent the main properties of the muscle, tendon, aponeurosis such as their length, activation signal, contraction velocity and exerted force. These are parameters that represent e.g. mechanical properties of them.

Since the natural muscle has got a hierarchical structure, it is straightforward to use a hierarchical model structure. Each main parts of the muscle will equal a level of the hierarchical model.

The model described in this report is a 2D model for the sake of simplicity. We plan the realization of 3D model in the future, therefore we take into account this perspective during the planning.

1.2.2 Modelling aim

Our main aim is to create a general framework of limb model and analyze its properties. Using this framework e.g. different models of the same process should be tested easily. Using this limb model, we would like to simulate the movement of limbs, the contraction and force generation mechanisms of the muscles containing sarcomeres, fibers, tendon (and aponeurosis). In addition to the simulation we would like to investigate the sensitivity of model's output to its parameters and the interaction of levels.

1.2.3 The hierarchical structure of the problem

The multi-scale nature of a detailed limb model is a consequence of a wide range of mechanisms that contribute to the movement and can only be described on rather different scales of sizes:

- *chemical processes* on a microscopic (atomic) scale that convert chemical potential into forces,
- *bio-mechanical processes* that describe the force generation and addition on the biological cell and on the fiber scales,

- *force integration process* in muscle that realize the method how force of muscle is determined from the force of fibers taking into account the pennate muscle and passive characteristics
- *force transformation process via tendon* that describes the effect of tendon
- *joint rotation process* as the effect of exerted torque. It is determined by the dynamics of the skeleton and the size, location and activation of muscles
- *segment interaction process* on the level of limb that determine the effect of joint rotation into the remain joints and segments.

This model contains more levels modelling one or more important anatomical and/or physiological process of the limb and muscle [1, 8, 46, 47]. So this model is a multilevel model. In an average paper in limb modelling the reader can find the model of one of these levels.

One of the most important properties of our model is that any used sub-model can be replaced with another model of same process. It means that our model is modular. It means that the interfaces between levels are defined in a precise way and designed to be general.

The model contains four levels and one of the levels contains three sub-levels as depicted in Fig.1.1. The levels are as follows:

- *Level of sarcomere*: Sarcomere is the basic force generation unit in the muscle. It is responsible for the force generation according to its state and excitation. This level contains the molecular model of force generation and bio-chemical processes. In living muscle the strength of force depends on the length of sarcomere, velocity of contraction and frequency of exciting action potentials. These dependencies should be modelled this level. At the same time one or more of these dependencies are modelled in the next level. This level contains the parameters of the sarcomeres.
- *Level of motor unit or fiber*: The function of this level is the generation of force of motor unit from the forces of sarcomeres that are in the given motor unit. Here we assume that the motor unit contains the same muscle fibers and sarcomeres. This level defines those effects that influence the force generation but are not modelled in the level of sarcomere. This level defines some other effects such as passive forces.
- *Level of muscle*: This level computes the forces and torques of muscles. To complete this task, this level sums the forces of motor units that are in the given muscle, models the effect of tendon, aponeurosis and pennate muscles. This level contains the parameters of muscle such as PCSA, attachment points, etc. This level contains three sub-levels:
 - Sub-level of muscle: this sub-level sums the effects of motor units and pennate muscle.
 - Sub-level of tendon: this sub-level computes the effect of tendon.
 - Sub-level of aponeurosis: this sub-level computes the effect of aponeurosis.
- *Level of limb*: This level is responsible for the computation of the movement of limb if the torques of muscles of every joint are known. This level computes the joint angles, their velocities and their accelerations. It means that this level must solve the dynamic equations of the limb and it must determine the interaction effect of segments.

In this framework the interfaces between levels play important role. Interface between the level of sarcomere and the level of fiber contains four equation: the transformations of length, contraction velocity and frequency of fiber into the length, contraction velocity and frequency of sarcomere and the transformation of force of sarcomere into the force of fiber. Except for them same parameter computation is belong to the interface: computation of minimal, maximal, optimal length of fiber from the minimal, maximal and optimal length of sarcomere and the computation of maximal force of fiber from the maximal force of sarcomere.

The interface between the level of fiber and level of muscle, sub-level of muscle contains four equations: the transformation of length, contraction velocity and frequency of muscle into the length, contraction velocity and frequency of fiber and the transformation of the force of fiber into the force of muscle. There are some parameter transportation: the level of muscle has to know the value of maximal and minimal exciting frequency of the fiber, the physiological cross sectional area of the fiber and the recruitment order of the fiber.

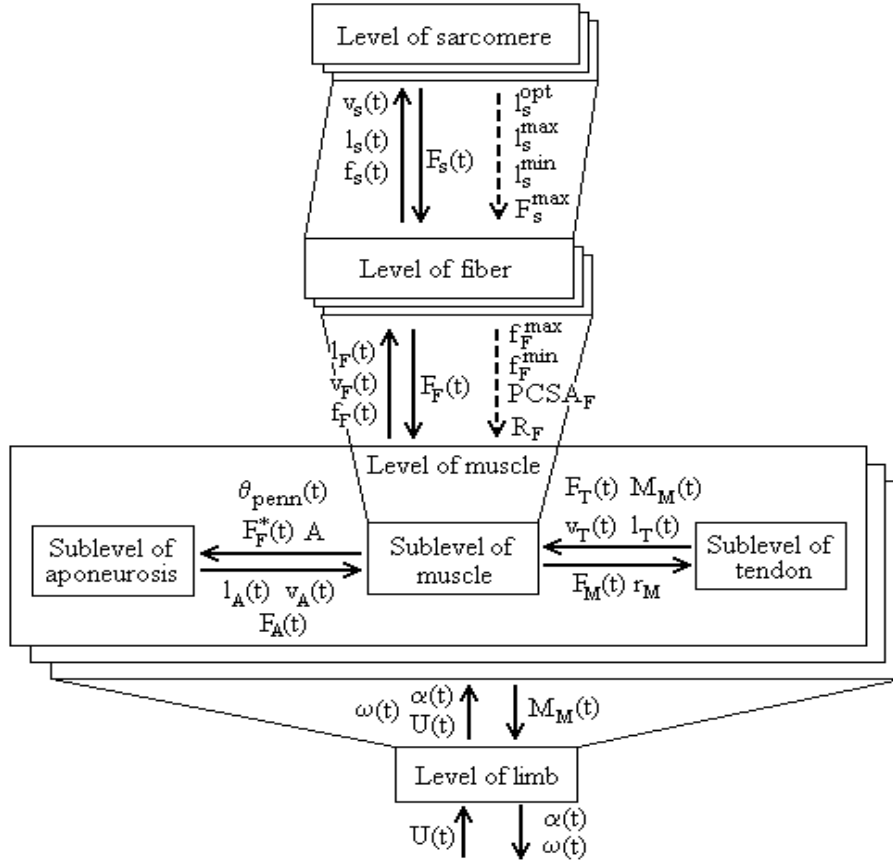


Figure 1.1: *Structure of model: model contains four levels and one level contains three sublevels. The dotted arrows mean the parameter transportation between levels, while the continuous arrows mean the transportation of variables between levels. The meaning of variables and parameters are found in detailed descriptions of the levels*

Interface between the level of muscle, sub-level of muscle and level of limb contains twice as many equations as joints, the transformation of joint angles and joint velocities into the sum of joint angles and joint velocities and vice versa. It also contains the transportation of joint torque from the sub-level of muscle to level of limb and the transportation of activation signal from the level of limb to the sub-level of muscle.

Interface between the level of muscle, sub-level of muscle and the level of muscle, sub-level of tendon contains the transportation of force of muscle and its moment arm from the sub-level of muscle to the sub-level of tendon and the transportation of the force of tendon, the torque of muscle, the length of tendon and the contraction velocity of tendon from the sub-level of tendon to the sub-level of muscle.

Interface between the level of muscle, sub-level of muscle and the level of muscle, sub-level of aponeurosis contains the transportation of the pennate angle, the sum of force of muscle's fibers, the length of the fiber and the area of the muscle from the sub-level of muscle to the sub-level of aponeurosis and the transportation of the length, the contraction velocity and the force of aponeurosis from the sub-level of aponeurosis to the sub-level of muscle.

1.2.4 Model parameters

In order to indicate the level or sub-level a model parameter belongs to, the following **indexing notation** is used throughout the report. The indexes are written at the bottom right position of an identifier, next to the index of parameters using coma between them. We use

- index q in the parameters and variables of sarcomeres,

- index i in the parameters and variables of motor units,
- index j in the parameters and variables of muscles and
- index k in the parameters and variables of segments and joints.

Thus we speak of the q^{th} sarcomere, i^{th} motor unit, j^{th} muscle and k^{th} segment or k^{th} joint, respectively. There are two different kinds of parameters:

- *Given parameter*: Their values are given by the user when he/she initializes the model.
- *Computed parameter*: Their value are computed by the computer from the initial values and given parameters. Their values must be computed at once in the beginning of simulation.

Other groups of parameters are

- *Model-independent*: These parameters are independent of the currently used model of the given level so they define general properties of the levels such as length of the muscle, maximum force of sarcomere etc. They occur in each model of the given process. These parameters are suitable and possible parameters of the interface.
- *Model-dependent*: a parameter depends on the model if it is defined by the currently used model and not by all model of the given process. If a model will be replaced with a new model of the same process, then the dependent parameters should be changed.

1.2.5 Inputs and outputs of the model

Both the inputs and the outputs of a model should be measurable signals, that is, time-varying quantities.

The input of the model consists of the activation signal or stimulating signal of each muscle. Activation signal is, for example, the envelope of the EMG signal. Activation signals are normalized, i.e. their value is between zero and one. The input signal should change in time, so it is a function of time.

The output of the model includes the joint angles, their velocities and accelerations (that together form a so called **movement pattern**) as a function of time.

1.2.6 Modelling assumptions

In order to obtain a realistic yet feasible model, we use a set of *simplifying modelling assumptions* in the phase of model building. These are in the form of constraints that must be satisfied by the model:

1. Active muscle force is influenced by length of the muscle, velocity of shortening and the muscle's excitation [9, 19, 28].
2. Moment arm: moment arms are constant and do not depend on the joint angles (possible development).
3. 2D: the limb, the muscles and the movement are in 2D.
4. Viscoelasticity: our model does not simulate the viscoelasticity of the muscle tissue, so the model of passive force will be simple. The energy storage cannot be simulated.
5. Aponeurosis: only the elastic property of aponeurosis is taken into account [40, 48].
6. Tendon: tendon is modelled using Voight model [9].
7. Connection between sarcomere and motor unit: there can be more different kinds of sarcomere in the model but a given motor unit contains only one kind of sarcomere.
8. Connection between motor unit and muscle: more different kinds of motor units can be in one muscle.
9. Connection between muscle and joint: more muscles can rotate the given joint in the same direction.
10. One joint muscle: our model deals with only one joint muscle. The effects of more joints muscles are omitted. [8, 36]

11. Geometry of muscle: geometry of muscles is linearized therefore the curvature and bulging of fibers and aponeurosis are neglected.[40], [41]
12. Area of the muscle: area of the muscle is constant during the contraction. It is the analogy of the constant volume of muscle during contraction. [37], [49]
13. Number of sarcomere connected serial and parallel: The numbers of serial connected and parallel connected sarcomeres are constants.
14. Fatigue and potentialization: we do not deal with the fatigue and muscle potentialization.
15. Force generation: force depends on the length of the muscle, its contraction velocity and the frequency of the applied EMG signal (input signal)
16. Passive force: Passive force is described in the level of motor unit.
17. Pennate muscle: models the effect of pennate muscle.
18. Chemical process: we do not deal with the modelling of chemical processes of muscle and sarcomere. We use constant values of concentration of chemical matters.
19. Number of segment and number of muscle in one joint are arbitrary.
20. Connection of segment is serial.
21. Short time histories of firing frequency, amount of shortening performed and velocity of shortening are not taken into account.
22. Recruitment is taken into account as in [3]

Chapter 2

Model development, description and solvability analysis

In this chapter the model equations of each level are described together with their variables and parameters. The value of the model parameters that can be found in the literature are also given.

We have to note that the models that are used in this chapter are only example models of the given processes except for the dynamic model of limb. It means that anybody can use another model of the given process using the same interfaces. Of course same analysis steps are valid only these models, so if someone would like to use an other model then he/she has to analyze this new model in similar way.

As a necessary preparatory step of the model solution, solvability analysis is also performed separately for the models in each level. This includes the analysis of the degree of freedom and the index of the models in the form of differential algebraic equation (DAE) system.

2.1 Sarcomere level

This model is responsible for the simulation of force generation at the level of sarcomere. The generated force depends on a number of factors such as length, velocity of contraction, the frequency of exciting action potential of the sarcomere and biochemical processes in the sarcomere. The structure of level of sarcomere can be seen in Fig.2.1.

2.1.1 Model equations

At present, we use the model of Derényi and Vicsek [5] as the model of sarcomere. This model deals only with the effect of contraction velocity to the force generation. So the effect of muscle length and frequency of input must be modelled in the level of motor unit. The model of Derényi and Vicsek does not contain any differential equations, it only contains algebraic equations. There can be only one model independent differential equation in this level: the contraction velocity of sarcomere is the time derivative of the length of the sarcomere, i.e.:

$$\frac{dl_{S,q}(t)}{dt} = -v_{S,q}(t)$$

This differential equation is not used directly in the model, but we use it to determine the expression of contraction velocity of sarcomere from the expression of the length of sarcomere. The sarcomere contraction velocity is positive if the length of sarcomere decreases. This is the reason of minus sign.

The algebraic equations form then the model of this level:

- Optimal, maximal and minimal length of sarcomere: These equations are given by [16]

$$l_{S,q}^{opt} = 2l_{actin,q} \tag{2.1}$$

$$l_{S,q}^{max} = l_{myosin,q} + 2l_{actin,q} \tag{2.2}$$

$$l_{S,q}^{min} = 0.9l_{myosin,q} \tag{2.3}$$

Level of sarcomere (S)

Generation of force of sarcomere takes into account the molecular effects if they are needed.

Variables	Parameters	Computed parameters
Model independent	Model independent	Model independent
$v_s(t)$ [m/s]	l_{myosin} [m]	l_s^{opt} [m]
$F_s(t)$ [N]	l_{actin} [m]	l_s^{max} [m]
— — —	Model dependent	l_s^{min} [m]
$l_s(t)$ [m]	k_{p-} [1/s] l [m]	F_s^{max} [N]
$f_s(t)$ [Hz]	k_{p+} [1/Ms] d [m]	Model dependent
Model dependent	$k_{\text{ADP-}}$ [1/s] δ [m]	τ_a [s]
—	$k_{\text{ADP+}}$ [1/Ms] [P] [M]	τ_d [s]
	$k_{\text{ATP+}}$ [1/Ms] [ADP] [M]	w [1]
	f [N] [ATP] [M]	
	f' [N]	

Figure 2.1: Structure of level of sarcomere. Meaning of variables and parameters are in the paragraph **Variables and parameters**

- Maximal force of sarcomere:

$$F_{S,q}^{\text{max}} = \frac{l_g}{d_q} f_q w_q \quad (2.4)$$

- Weight: computing of a weight:

$$w_q = \frac{k_{P-,q}}{k_{P-,q} + k_{P+,q} [P]_q} \quad (2.5)$$

- Maximal contraction velocity: it depends on molecular effect and concentration of different substrates.

$$V_q^{\text{max}} = V_q^{\text{max},\infty} \frac{[ATP]_q}{K_{m,q} + [ATP]_q} \quad (2.6)$$

where

$$K_{m,q} = K_{m,q}^0 \left(1 + \frac{[ADP]_q}{K_{i,q}} \right) \quad (2.7)$$

$$V_q^{\text{max},\infty} = \frac{f_q}{f'_q} l_q k_{\text{ADP-},q} \quad (2.8)$$

$$K_{m,q}^0 = \frac{k_{\text{ADP-},q}}{k_{\text{ATP+},q}} \quad (2.9)$$

$$K_{i,q} = \frac{k_{\text{ADP-},q}}{k_{\text{ADP+},q}} \quad (2.10)$$

- Normalization of contraction velocity:

$$v_{S,q}^{\text{norm}} = \frac{v_{S,q}}{1.15 V_q^{\text{max}}} \quad (2.11)$$

- Force of sarcomere: currently generated force of q^{th} sarcomere is

$$F_{S,q}(v_{S,q}) = \frac{l_q}{d_q} f_q w_q \left(1 - e^{-\frac{0.15}{v_{S,q}^{\text{norm}}}} \right) * \left[1 - \frac{\delta_q}{l_q} \left(\frac{v_{S,q}^{\text{norm}}}{0.15} - \frac{1}{e^{\frac{0.15}{v_{S,q}^{\text{norm}}}} - 1} \right) - v_{S,q}^{\text{norm}} \right] \quad (2.12)$$

This characteristic is displayed in fig.2.2.

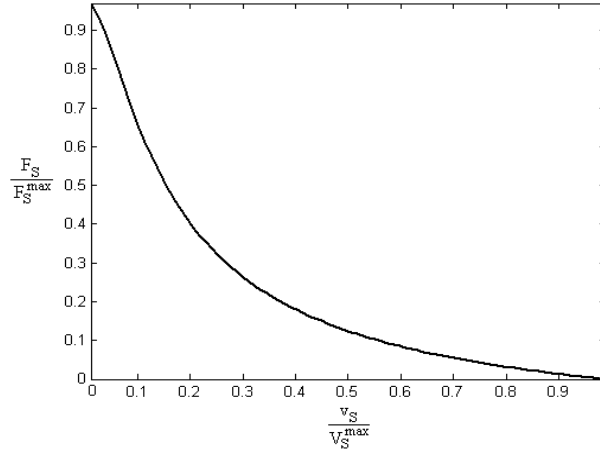


Figure 2.2: Force of sarcomere as a function of contraction velocity according to [5]

Variables and parameters of this level are:

- Model independent variables
 - $v_S(t)$ [m/s]: contraction velocity of sarcomere. It is positive if the length of sarcomere is decreasing.
 - $F_S(t)$ [N]: generated force of sarcomere.
 - $l_S(t)$ [m]: length of sarcomere. It is not used in this model.
 - $f_S(t)$ [Hz]: frequency of action potential. It is not used in this model.
- Model dependent variables: there are not model independent variables.
- Model independent parameters
 - l_{myosin} [m]: length of myosin filament.
 - l_{actin} [m]: length of actin filament.
- Model dependent parameters
 - k_{P-} [1/s]: dissociation rate constant of P to make the strong bind between actin and myosin.
 - k_{P+} [1/Ms]: association rate constant of P to the AM complex (actin-myosin complex).
 - k_{ADP-} [1/s]: dissociation rate constant of ADP . It means the speed of dissociation of ADP from AM complex to make free space for ATP .
 - k_{ADP+} [1/Ms]: association rate constant of ADP to the AM complex.
 - k_{ATP+} [1/Ms]: association rate constant of ATP to the AM complex. It initializes the detachment of AM complex.
 - f [N]: force of attachment of myosin and action. This force is generated by myosin head in the power-stroke region.
 - f' [N]: force of detachment of AM complex. This force is generated by myosin head in the drag-stroke region.
 - l [m]: working distance of power-stroke.
 - d [m]: distance between two neighbouring binding sites.
 - δ [m]: Debye length of cross-bridge.
 - $[P]$ [M]: concentration of P .
 - $[ADP]$ [M]: concentration of ADP .

- $[ATP]$ [M]: concentration of ATP .
- Model independent, computed parameters
 - l_S^{opt} [m]: optimal length of sarcomere. Sarcomere can generate the maximal force at this length.
 - l_S^{max} [m]: maximal length of sarcomere.
 - l_S^{min} [m]: minimal length of sarcomere.
 - F_S^{max} [N]: maximal force of sarcomere. Now it is not need for the simulation.
- Model dependent, computed parameters
 - w [1]: steady state probability of strongly bound state which is approached exponentially.
 - $V_q^{max,\infty}$ [m/s]: is the estimation of the maximal contraction velocity if $[ATP] = \infty$.

2.1.2 Value of parameters

This part gives the value of parameters if they can be found in the literature with a pointer to their reference. The notation *psmR* means psoasmuscle in rabbit, while *smmR* means semimembranous in rabbit. If it is not indicated otherwise, the value is valid for humans.

Parameter	Value	Source
l_{myosin}	1.6 μ m	[8]
l_{actin}	1.35 μ m	[8] , [16]
k_{P-}	76 1/s (<i>psmR</i>) 25 1/s (<i>smmR</i>)	[5]
k_{P+}	0 1/Ms, 3100 1/Ms	[5]
k_{ADP-}	230 1/s (<i>psmR</i>) 76 1/s (<i>smmR</i>)	[5]
k_{ADP+}	0 1/Ms, 3.5 * 10 ⁵ 1/Ms	[5]
k_{ATP+}	0.76 1/ μ Ms (<i>psmR</i>) 3.8 1/ μ Ms (<i>smmR</i>)	[5]
f	4 pN	[5]
f'	4 pN	[5]
l	11 nm	[5]
d	45 nm	[8]
δ	3 nm	[5]
$[P]$	0 M, 12 mM	[5]
$[ADP]$	0 M, 0.8 mM	[5]
$[ATP]$	3 mM	[5]

2.1.3 Analysis of degree of freedom

In general there are four variables in the level of sarcomere. There are the length, the contraction velocity, the exciting signal and the currently generated force of sarcomere. But the first three variables are *dummy* variables determined in the next level, and this level get them as an input if they are necessary for the computation of level of sarcomere. Only the currently generated force of sarcomere is computed in this level. So the degree of freedom of this level is 0.

2.1.4 Analysis of the differential index of DAE

Differential equation is not used during the simulation in the level of sarcomere, there are only algebraic equations. The structure matrix can be seen in the table below. We note that the variable or parameter in the () bracket means that this variable or parameter is defined in other level and not the currently investigated level. So this variable must be the one of the input of currently investigated level. We also note, that the constant parameters of this level are not in the table and sign \times means that the current variable, parameter is in the current equation while \otimes means that the current equation defines the current variable or parameter. The sign (\times) means that this connection depends on the used model of sarcomere.

Level of motor unit or fiber (F)

Generates the force of fiber or motor unit from the force of sarcomere of the fiber.
 Compute passive force.

Variables	Parameters	Computed parameters
Model independent	Model independent	Model independent
$l_F(t)$ [m]	N_s [1]	l_F^{opt} [m]
$v_F(t)$ [m/s]	N_p [1]	l_F^{max} [m]
$f_F(t)$ [Hz]	f_{max} [Hz]	l_F^{min} [m]
$F_F(t)$ [N]	f_{min} [Hz]	F_F^{max} [N]
Model dependent	Model dependent	Model dependent
$l_F^{norm}(t)$ [1]	Force-length	—
$f_F^{norm}(t)$ [1]	ω [1]	Passive force
	β [1]	l_F^{slack} [1]
	ρ [1]	Recruitment
	Force-frequency	R_F [1]
	f_{th} [1]	
	k_{tan} [1]	

Figure 2.3: Structure of level of motor unit or fiber. Meaning of variables and parameters are in the paragraph **Variables and parameters**

	l_S^{opt}	l_S^{max}	l_S^{min}	F_S^{max}	w	$F_S(t)$	$(l_S(t))$	$(v_S(t))$	$(f_S(t))$
(2.1)	⊗								
(2.2)		⊗							
(2.3)			⊗						
(2.4)				⊗					
(2.5)					⊗				
(2.12)					×	⊗	(×)	×	(×)

The table shows that each algebraic variable and parameter that must be defined in this level has got an equation assigned to it. It means that the index of this sub-model is equal to 1.

2.2 Motor unit level

The model on the level of motor unit describes the muscle fibers and the motor unit composed therefrom. The main difference between them is that motor unit contains more muscle fibers of the same kind. Following the notation convention, F in the index is used to identify the variables and parameters of this level.

The level of motor unit is responsible for the integration of forces of sarcomere producing the given motor unit. This level provides data to the level of sarcomere and uses the forces of sarcomeres, integrates them and delivers these data to the level of muscle.

This level models the effects of force generation that are not modelled on the level of sarcomere. Since we use a model of sarcomeres which models only the effect of contraction velocity, the level of motor unit must model the effect of length of muscle (sarcomere) and the effect of exciting action potentials.

The structure of level of motor unit can be seen in Fig. 2.3.

2.2.1 Model equations

There is one differential equation in this level:

$$\frac{dl_{F,i}(t)}{dt} = -v_{F,i}(t)$$

This differential equation is not used directly in the model, but we use it to determine the expression of contraction velocity of fiber from the expression of the length of fiber.

The constitutive algebraic equations are the ones that are used for the computations performed at this level.

- Interface with the level of sarcomere: these computations are completed to that sarcomeres what form the given fiber, motor unit i.e. q_{th} sarcomere are in the i_{th} fiber, motor unit.

- Computing of length of sarcomere from the length of fibers:

$$l_{S,q}(t) = \frac{l_{F,i}(t)}{N_{s,i}} \quad (2.13)$$

- Computing of contraction velocity of sarcomere

$$v_{S,q}(t) = \frac{v_{F,i}(t)}{N_{s,i}} \quad (2.14)$$

- Computing of exciting input of sarcomere

$$f_{S,q}(t) = f_{F,i}(t) \quad (2.15)$$

- Computing of computed parameters: computing of optimal, maximal, minimal length of fiber and the maximal force of the fiber from the same data of sarcomere. Data of sarcomere are given from the level of sarcomere.

$$l_{F,i}^{opt} = N_{s,i} l_{S,q}^{opt} \quad (2.16)$$

$$l_{F,i}^{max} = N_{s,i} l_{S,q}^{max} \quad (2.17)$$

$$l_{F,i}^{min} = N_{s,i} l_{S,q}^{min} \quad (2.18)$$

$$F_{F,i}^{max} = N_{p,i} F_{S,q}^{max} \quad (2.19)$$

- Normalization of length of fiber

$$l_{F,i}^{norm}(t) = \begin{cases} \frac{l_{F,i}(t) - l_{F,i}^{min}}{l_{F,i}^{opt} - l_{F,i}^{min}} & \text{if } l_{F,i}(t) \leq l_{F,i}^{opt} \\ \frac{l_{F,i}(t) - l_{F,i}^{opt}}{l_{F,i}^{max} - l_{F,i}^{opt}} + 1 & \text{if } l_{F,i}(t) > l_{F,i}^{opt} \end{cases} \quad (2.20)$$

- Normalization of exciting frequency

$$f_{F,i}^{norm}(t) = \frac{f_{F,i}(t) - f_{F,i}^{min}}{f_{F,i}^{max} - f_{F,i}^{min}} \quad (2.21)$$

- *Force-length of muscle* characteristic [3]

$$FL_i(l_{F,i}^{norm}) = e^{-\left| \frac{(l_{F,i}^{norm})^{\beta_i} - 1}{\omega_i} \right|^{\rho_i}} \quad (2.22)$$

This characteristic is showed in fig.2.4.

- *Force-exciting frequency* characteristic: sigmoid function represent this characteristic.

$$FF_i(f_{F,i}^{norm}) = \frac{a}{1 + e^{-\frac{f_{F,i}^{norm} - f_{th,i}}{k_{tan,i}}}} + b \quad (2.23)$$

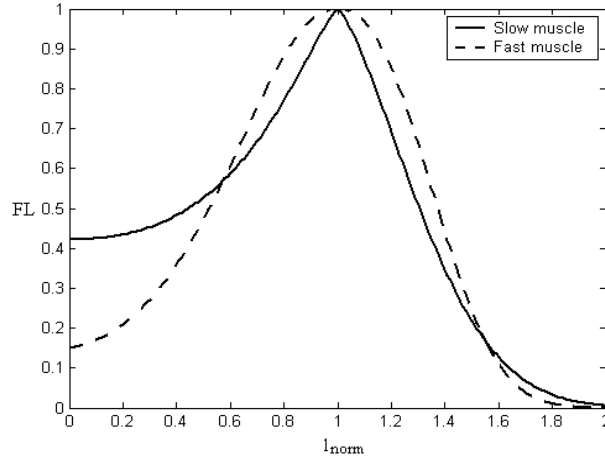


Figure 2.4: Force-length characteristic

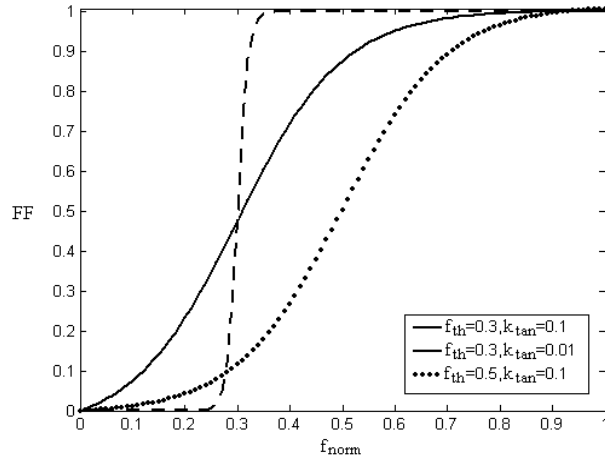


Figure 2.5: Force-frequency characteristic in case of different parameters.

where

$$a = - \frac{\left(1 + e^{-\frac{1-f_{th,i}}{k_{tan,i}}}\right) \left(1 + e^{\frac{f_{th,i}}{k_{tan,i}}}\right)}{e^{\frac{f_{th,i}}{k_{tan,i}}} \left(e^{-\frac{1}{k_{tan,i}}} - 1\right)}$$

and

$$b = \frac{1 + e^{-\frac{1-f_{th,i}}{k_{tan,i}}}}{e^{\frac{f_{th,i}}{k_{tan,i}}} \left(e^{-\frac{1}{k_{tan,i}}} - 1\right)}$$

This characteristic is showed in fig.2.5.

- Passive force [4]

$$F_{PE,i}(l_{F,i}^{norm}) = \begin{cases} \frac{1}{(2-l_{F,i}^{slack})^2} (l_{F,i}^{norm} - l_{F,i}^{slack})^2 & \text{if } l_{F,i}^{norm} > l_{F,i}^{slack} \\ 0 & \text{if } l_{F,i}^{norm}(t) \leq l_{F,i}^{slack} \end{cases} \quad (2.24)$$

- Force of fiber, motor unit

$$F_{F,i}(t) = F_{S,q}(v_{S,q}) N_{p,i} FL_i(l_{F,i}^{norm}) FF_i(f_{F,i}^{norm}) + F_{PE,i}(l_{F,i}^{norm}) F_{PE,i}^{max} \quad (2.25)$$

Variables and parameters of this level are:

- Model independent variables:
 - $v_F(t)$ [m/s]: contraction velocity of fiber. It is positive if the length of fiber is decreasing.
 - $F_F(t)$ [N]: force generated by fiber.
 - $l_F(t)$ [m]: length of fiber.
 - $f_F(t)$ [Hz]: frequency of exciting action potential of fiber.
- Model dependent variables:
 - $l_F^{norm}(t)$ [1]: normalized length of fiber. Its value is between 0 and 2. The optimal length of muscle is 1 in normal value.
 - $f_F^{norm}(t)$ [1]: normalized frequency of exciting action potential of fiber. Its value is between 0 and 1.
- Model independent parameters:
 - N_s [1]: number of serial connected sarcomere in the given fiber.
 - N_p [1]: number of parallel connected sarcomere in the given fiber.
 - f_{max} [Hz]: maximal frequency of exciting action potential.
 - f_{min} [Hz]: minimal frequency of exciting action potential.
 - $PCSA_F$ [m²]: physiological cross sectional area of fiber.
 - F_{PE}^{max} [N]: maximal passive force.
- Model dependent parameters:
 - ω [1]: first parameter of *force-length of muscle* characteristic.
 - β [1]: second parameter of *force-length of muscle* characteristic.
 - ρ [1]: third parameter of *force-length of muscle* characteristic.
 - f_{th} [1]: first parameter of *force-frequency* characteristic. It means that normalized frequency where the half of the maximal force can be produced.
 - k_{tan} [1]: second parameter of *force frequency* characteristic. It gives the tangential value of the characteristic in the vicinity of point of f_{th} .
 - l_F^{slack} [1]: parameter of passive force, the passive slack length of the fiber. It means that normalized length of fiber where the passive force begin the increasing from the zero. Its value is between 0 and 2 and 1 means the optimal length.
 - R_F [1]: recruitment order of the fiber. It means that the greater and greater excitement are the more and more fibers generate force. This number give the serial number of the given fibers. The fiber generates force if every fibers having less ordered number have generated force already.
- Model independent computed parameters:
 - l_F^{opt} [m]: optimal length of fiber.
 - l_F^{max} [m]: maximal length of fiber.
 - l_F^{min} [m]: minimal length of fiber.
 - F_F^{max} [N]: maximal force generated by fiber.
- Model dependent computed parameters: none

2.2.2 Value of parameters

The value of parameters that can be found in the literature are listed below with notation of their reference.

Parameter	Value	Source
N_s	depend on the muscle, $10^2 - 10^4$	[8]
N_p	depend on the muscle, $10^{13} - 10^{14}$	[8]
f_{max}	depend on the muscle	[8]
f_{min}	depend on the muscle	[8]
$PCSA_F$	depend on the muscle	[8], [47], MRI
F_{PE}^{max}	depend on the muscle	
ω	1.12 for slow m. 0.75 for fast m.	[3]
β	2.3 for slow m. 1.55 for fast m.	[3]
ρ	1.61 for slow m. 2.21 for fast m.	[3]
f_{th}	unknown, dep. on m.	
k_{tan}	unknown, dep. on m.	
l_F^{slack}	unknown, dep. on m.	
R_F	unknown, dep. on m.	

2.2.3 Analysis of degree of freedom

There are 13 variables and parameters what must be defined in the level of motor unit. There are 13 equation in this level: (2.13)-(2.25). It means that the degree of freedom of the level of motor unit is 0.

2.2.4 Analysis of the differential index of DAE

Differential equation is not used during the simulation in the level of motor unit, there are only algebraic equations. The structure matrix can be seen in the table below. We note that the variable or parameter in the () bracket means that this variable or parameter is defined in another level. So this variable is one of the inputs of currently investigated level.

We also note, that the constant parameters of this level are not in the table and sign \times means that the current variable, parameter is in the current equation while \otimes means that the current equation defines the current variable or parameter.

	$l_S(t)$	$v_S(t)$	$f_S(t)$	l_F^{opt}	l_F^{max}	l_F^{min}	F_F^{max}	$l_F^{norm}(t)$	$f_F^{norm}(t)$	FL	FF
(2.13)	\otimes										
(2.14)		\otimes									
(2.15)			\otimes								
(2.16)				\otimes							
(2.17)					\otimes						
(2.18)						\otimes					
(2.19)							\otimes				
(2.20)				\times	\times	\times		\otimes			
(2.21)									\otimes		
(2.22)								\times		\otimes	
(2.23)									\times		\otimes
(2.24)								\times			
(2.25)							\times			\times	\times

	F_{PE}	$F_F(t)$	$(F_S(t))$	$(l_F(t))$	$(v_F(t))$	$(f_F(t))$	l_S^{opt}	(l_S^{max})	l_S^{min}	(F_S^{max})
(2.13)				×						
(2.14)					×					
(2.15)						×				
(2.16)							×			
(2.17)								×		
(2.18)									×	
(2.19)										×
(2.20)				×						
(2.21)						×				
(2.22)										
(2.23)										
(2.24)	⊗									
(2.25)	×	⊗	×							

The table shows that each algebraic variable and parameter that is computed in this level has got an equation associated to it. It means, that the differential index is equal to 1.

2.3 Level of muscle

This level is responsible for the integration of the effect of fibers composing the given muscle. In addition, the level of muscle is responsible for the computing and modelling of effects of pennate muscles, tendons and aponeurosis.

Because pure muscle, tendon and aponeurosis can be modelled separately, three sub-levels are defined to complete these tasks:

- Sub-level of muscle: integrates the forces of fibers composing the given muscle. It computes the length and contraction velocity of the muscle. It is responsible for the simulation of the effect of pennate muscle.
- Sub-level of tendon: model of the dynamics of tendon. It computes the force of tendon, length of tendon, contraction velocity of tendon.
- Sub-level of aponeurosis: model of aponeurosis. It computes the length, contraction velocity and force of aponeurosis.

We use the index M for sign the variables and parameters of the muscle without tendon and aponeurosis. Similarly, index A and index T is used to sign the variables and parameters of aponeurosis and tendon, respectively.

During computation we suppose that the i_{th} fiber composes the j_{th} muscle. Mathematical expression $i \in j$ means this condition.

For simulate the pennate effect, we use the model of Linden [40], [41] with a little modification: a differential equation describes the properties of aponeurosis and not a algebraic one, but the *length-force* characteristic of the aponeurosis is the same. This modification modify the exact expression of pennate angle from the area of the muscle, but the main properties is the same.

In order to specifying the structure of the muscle level we give the structure of the sub-levels separately. The structure of sub-level of muscle can be seen in Fig.2.6., while the structure of sub-level of tendon can be seen in Fig.2.7., and finally the structure of sublevel of aponeurosis can be seen in Fig.2.8.

2.3.1 Model equations

The differential equations of this level are as follows:

Level of muscle, sublevel of muscle

Computes the force of the pure muscle, computes the effect of pennate muscle

Variables	Parameters	Computed parameters
Model independent	Model independent	Model independent
$l_M(t)$ [m]	U_M^{th} [1]	F_M^{max} [N]
$v_M(t)$ [m/s]	r_M [m]	$PCSA_M$ [m ²]
$U_M(t)$ [1]	d_M^{dist} [m]	
$F_M(t)$ [N]	d_M^{prox} [m]	
$\bar{M}_M(t)$ [Nm]	A [m ²]	Model dependent
Pennate	Model dependent	—
Θ_{penn} [rad]	—	
$F_F^*(t)$ [N]		
Model dependent		
$l_{M+T}(t)$ [m]		
$v_{M+T}(t)$ [m/s]		
$\alpha_{FM}(t)$ [rad]		
$\beta_{AM}(t)$ [rad]		

Figure 2.6: Structure of sub-level of muscle. Meaning of variables and parameters are in the paragraph *Variables and parameters*

- Sub-level of muscle:

$$\frac{dl_{M+T,j}(t)}{dt} = -v_{M+T,j}(t) \quad (2.26)$$

$$\frac{dl_{M,j}(t)}{dt} = -v_{M,j}(t) \quad (2.27)$$

$$\frac{dl_{F,i}(t)}{dt} = -v_{F,i}(t) \quad (2.28)$$

$$\frac{d\theta_{penn,j}(t)}{dt} = \left(\frac{v_{F,i}(t)}{l_{F,i}(t)} - \frac{v_{A,j}(t)}{l_{A,j}(t)} \right) \tan \theta_{penn,j}(t) \quad (2.29)$$

- Sub-level of tendon:

$$\frac{dl_{T,j}(t)}{dt} = \begin{cases} -\frac{D_{T,j}(l_{T,j}(t)-l_{T,j}^{slack})+F_{T,j}(t)}{C_{T,j}} & \text{if } l_{T,j}(t) \geq l_{T,j}^{slack} \\ 0 & \text{otherwise} \end{cases} \quad (2.30)$$

$$\frac{dl_{T,j}(t)}{dt} = v_{T,j}(t) \quad (2.31)$$

- Sub-level of aponeurosis

$$\frac{dl_{A,j}(t)}{dt} = \begin{cases} -\frac{C_{A,j}(l_{A,j}(t)-l_{A,j}^{slack})^2+F_{A,j}(t)}{V_{A,j}} & \text{if } l_{A,j}(t) \geq l_{A,j}^{slack} \\ 0 & \text{otherwise} \end{cases} \quad (2.32)$$

$$\frac{dl_{A,j}(t)}{dt} = v_{A,j}(t) \quad (2.33)$$

The algebraic equations are:

- Sub-level of muscle:

– Connection with the level of motor unit:

Level of muscle, sublevel of tendon (T)

Computes the force of tendon and torque of the muscle tendon complex

Variables	Parameters	Computed parameters
Model independent	Model independent	Model independent
$l_T(t)$ [m]	—	—
$v_T(t)$ [m/s]		
$F_T(t)$ [N]		
$M_M(t)$ [Nm]	Model dependent	
Model dependent	D_T [N/m]	Model dependent
—	C_T [Ns/m]	—
	l_T^{slack} [m]	

Figure 2.7: Structure of sub-level of tendon. Meaning of variables and parameters are in the paragraph *Variables and parameters*

Level of muscle, sublevel of aponeurosis (A)

Compute the force, length and contraction velocity of aponeurosis.

Variables	Parameters	Computed parameters
Model independent	Model independent	Model independent
$l_A(t)$ [m]	—	—
$v_A(t)$ [m/s]		
$F_A(t)$ [N]		
Model dependent	Model dependent	Model dependent
—	l_A^{slack} [m]	—
	C_A [N/m ²]	

Figure 2.8: Structure of sub-level of aponeurosis. Meaning of variables and parameters are in the paragraph *Variables and parameters*

- * Computation of length of fibers from the length of muscle [40]:

$$l_{F,i}(t) = \sqrt{l_{A,j}^2(t) (\cos^2 \theta_{penn,j}(t) + l_{M,j}^2(t)) - l_{A,j} \cos \theta_{penn,j}} \quad (2.34)$$

- * Computation of contraction velocity of fiber from the data of muscle:

$$v_{F,i}(t) = \frac{2l_{A,j}(t)v_{A,j}(t) \sin^2 \theta_{penn,j}(t) + l_{A,j}^2(t) \sin 2\theta_{penn,j}(t) \dot{\theta}_{penn,j}(t) + 2l_{M,j}(t)v_{M,j}(t)}{2(l_{F,i}(t) + l_{A,j}(t) \cos \theta_{penn,j})} + v_{A,j}(t) \cos \theta_{penn,j}(t) - l_{A,j}(t) \sin \theta_{penn,j} \dot{\theta}_{penn,j}(t) \quad (2.35)$$

- * Computation of exciting frequency of fiber from the activation signal of the muscle [3]:

$$f_{F,i}(t) = \begin{cases} \frac{f_{F,i}^{max} - f_{F,i}^{min}}{1 - U_{th,i,j}} [U_j(t) - U_{th,i,j}] + f_{F,i}^{min} & \text{if } U_j(t) \geq U_{th,i,j} \\ 0 & \text{otherwise} \end{cases} \quad (2.36)$$

where

$$U_{th,i,j} = \frac{\sum_{x=1}^i o(PCSA_{F,x})}{PCSA_{M,j}} U_{th,j}$$

i.e. $U_{th,i,j}$ is the activation threshold value of fiber i^{th} in the muscle j^{th} and $o(PCSA_{F,x})$ sort the fibers composing the given muscle in ascending order according to their recruitment order and gives fiber's PCSA in this order as output.

- * Sum of the force generated by the fibers (magnitude of force in the line of fibers)

$$F_{F,j}^*(t) = \sum_{i \in j} F_{F,i}(t) \quad (2.37)$$

- Force of muscle without tendon and aponeurosis [40]:

$$F_{M,j}(t) = F_{F,j}^*(t) \frac{\cos(\theta_{penn}(t))}{\cos(\beta_{AM,j}(t))} \quad (2.38)$$

- Pennate angle [40]

$$\theta_{penn,j}(t) = \alpha_{FM,j}(t) + \beta_{AM,j}(t) \quad (2.39)$$

- Angle between the aponeurosis and line of the exerted force [40]:

$$\beta_{AM,j}(t) = \arcsin\left(\frac{l_{F,i}(t)}{l_{M,j}(t)} \sin \theta_{penn,j}(t)\right) \quad (2.40)$$

- Angle between the fibers and line of the exerted force [40]:

$$\alpha_{FM,j}(t) = \arcsin\left(\frac{l_{A,j}(t)}{l_{M,j}(t)} \sin \theta_{penn,j}(t)\right) = \theta_{penn,j}(t) - \beta_{AM,j}(t) \quad (2.41)$$

- Physiological cross-section area of the muscle

$$PCSA_{M,j} = \sum_{i \in j} PCSA_{F,i} \quad (2.42)$$

- The length of muscle-tendon complex as a function of joint angles. The j^{th} muscle rotates the k^{th} joint:

- * Extensor muscle: it increases the joint angle.

$$l_{M+T,j}(t) = \sqrt{r_{M,j}^2 + (d_{M,j}^{prox})^2 + 2r_{M,j}d_{M,j}^{prox} \sin \frac{\alpha_k(t)}{2}} + \sqrt{r_{M,j}^2 + (d_{M,j}^{dist})^2 + 2r_{M,j}d_{M,j}^{dist} \sin \frac{\alpha_k(t)}{2}} \quad (2.43)$$

- * Flexor muscle: it decreases the joint angle

$$l_{M+T,j}(t) = \sqrt{r_{M,j}^2 + (d_{M,j}^{prox})^2 - 2r_{M,j}d_{M,j}^{prox} \sin \frac{\alpha_k(t)}{2}} + \sqrt{r_{M,j}^2 + (d_{M,j}^{dist})^2 - 2r_{M,j}d_{M,j}^{dist} \sin \frac{\alpha_k(t)}{2}} \quad (2.44)$$

- The contraction velocity of muscle-tendon complex according to the (2.26) and (2.43)-(2.44) is:

- * Extensor muscle

$$v_{M+T,j}(t) = - \frac{r_{M,j}d_{M,j}^{prox} \left(\cos \frac{\alpha_k(t)}{2}\right) \frac{\omega_k(t)}{2}}{\sqrt{r_{M,j}^2 + (d_{M,j}^{prox})^2 + 2r_{M,j}d_{M,j}^{prox} \sin \frac{\alpha_k(t)}{2}}} - \quad (2.45)$$

$$- \frac{r_{M,j}d_{M,j}^{dist} \left(\cos \frac{\alpha_k(t)}{2}\right) \frac{\omega_k(t)}{2}}{\sqrt{r_{M,j}^2 + (d_{M,j}^{dist})^2 + 2r_{M,j}d_{M,j}^{dist} \sin \frac{\alpha_k(t)}{2}}} \quad (2.46)$$

* Flexor muscle

$$v_{M+T,j}(t) = \frac{r_{M,j}d_{M,j}^{prox} \left(\cos \frac{\alpha_k(t)}{2} \right) \frac{\omega_k(t)}{2}}{\sqrt{r_{M,j}^2 + \left(d_{M,j}^{prox} \right)^2 - 2r_{M,j}d_{M,j}^{prox} \sin \frac{\alpha_k(t)}{2}}} + \quad (2.47)$$

$$+ \frac{r_{M,j}d_{M,j}^{dist} \left(\cos \frac{\alpha_k(t)}{2} \right) \frac{\omega_k(t)}{2}}{\sqrt{r_{M,j}^2 + \left(d_{M,j}^{dist} \right)^2 - 2r_{M,j}d_{M,j}^{dist} \sin \frac{\alpha_k(t)}{2}}} \quad (2.48)$$

– Length of muscle without tendon from the length of muscle-tendon complex and length of tendon:

$$l_{M,j}(t) = l_{M+T,j}(t) - l_{T,j}(t) \quad (2.49)$$

– Contraction velocity of the muscle without tendon from the contraction velocity of muscle-tendon complex and contraction velocity of tendon:

$$v_{M,j}(t) = v_{M+T,j}(t) + v_{T,j}(t) \quad (2.50)$$

– Conversion between the area of muscle and the pennate angle of muscle:

* Computation the pennate angle from the area of muscle based on [40] and [41]:

$$\sin^2 \theta_{penn,j}(t) = A_j \frac{l_{M,j}(t)^2 + l_{A,j}(t)^2 + 2\sqrt{l_{M,j}(t)^2 l_{A,j}(t)^2 - A_j^2}}{l_{A,j}(t)^2 \left([l_{M,j}(t)^2 - l_{A,j}(t)^2]^2 + 4A_j^2 \right)} \quad (2.51)$$

* Computation the area of muscle from the pennate angle of muscle based on [40] and [41]:

$$A_j = -\sin \theta_{penn,j}(t) \cos \theta_{penn,j}(t) l_{A,j}(t)^2 + \sin \theta_{penn,j}(t) l_{A,j}(t) \sqrt{\cos^2 \theta_{penn,j}(t) l_{A,j}(t)^2 + l_{M,j}(t)^2 - l_{A,j}(t)^2} \quad (2.52)$$

• Sub-level of tendon:

– Force of tendon:

$$F_{T,j}(t) = -F_{M,j}(t) \quad (2.53)$$

– Torque generates by tendon to rotate joint:

$$M_{M,j}(t) = -F_{T,j}(t)r_{M,j} \quad (2.54)$$

• Sub-level of aponeurosis:

– Force of aponeurosis [40]:

$$F_{A,j}(t) = -F_{F,j}^*(t) \cos(\theta_{penn,j}(t)) \quad (2.55)$$

The variables and parameters of this level are:

• Sub-level of muscle

– Model independent variables

* $v_M(t)$ [m/s]: contraction velocity of muscle without tendon. It is positive if the muscle contracts, i.e when the length of muscle is decreasing. It is the reason of minus sign in the differential equation (2.26).

* $F_M(t)$ [N]: generated force of muscle without tendon.

* $l_M(t)$ [m]: length of muscle without tendon.

* $F_F^*(t)$ [rad]: force of muscle at the line of fibers.

* $l_{M+T}(t)$ [m]: length of muscle-tendon complex.

- * $v_{M+T}(t)$ [m/s]: contraction velocity of muscle-tendon complex. It is positive if the muscle-tendon complex contracts, i.e when the length of muscle-tendon complex is decreasing.
- * $\theta_{penn}(t)$ [rad]: pennate angle of muscle. It means the angle between the line of aponeurosis and the line of fiber.
- Model dependent variables:
 - * $\alpha_{FM}(t)$ [rad]: angle between the fibers and line of the exerted force of muscle.
 - * $\beta_{AM}(t)$ [rad]: angle between the aponeurosis and line of the exerted force of muscle.
- Model independent parameters
 - * U_M^{th} [1]: threshold activation level of muscle. If the activation input of muscle is greater than this value, than the muscle generates force.
 - * r_M [m]: moment arm of the muscle.
 - * d_M^{dist} [m]: distance between the distant attachment point and the rotated joint.
 - * d_M^{prox} [m]: distance between the proximal attachment point and the rotated joint.
 - * A [m²]: area (or volume in 3D) of the muscle. Since in this model the area of the muscle plays role in the computing of pennate effect sometimes this parameter is referred as a parameter of the aponeurosis.
- Model dependent parameters: there are not such kind of parameters.
- Model independent computed parameters
 - * F_M^{max} [N]: maximal force of muscle in the line of muscle-tendon complex. Now it is not used.
 - * $PCSA_M$ [m²]: physiological cross-section area of the muscle.
- Model dependent computed parameters: there are not such kind of parameters.
- Sub-level of tendon
 - Model independent variables
 - * $l_T(t)$ [m]: length of tendon.
 - * $v_T(t)$ [m]: contraction velocity of tendon. it is positive if the length of tendon is increasing.
 - * $F_T(t)$ [N]: force generated by tendon.
 - * $M_M(t)$ [Nm]: torque of tendon to the joint.
 - Model dependent variables: none
 - Model independent parameters: none
 - Model dependent parameters
 - * l_T^{slack} [m]: length of tendon in rest. The tendon exert force if its length is greater or equal than its resting length.
 - * D_T [N/m]: spring constant of the tendon.
 - * C_T [Ns/m]: effect of contraction velocity to the force of tendon. Since the force of tendon is greater when the length of tendon is increasing than when it is decreasing, the sign of C_T is determined by the $C_T v_T \geq 0$ during lengthening of tendon.
 - Model independent computed parameters: none
 - Model dependent computed parameters: none
- Sub-level of aponeurosis
 - Model independent variables
 - * $l_A(t)$ [m]: length of aponeurosis.
 - * $v_A(t)$ [m]: contraction velocity of aponeurosis. It is positive if the length of aponeurosis is increasing.
 - * $F_A(t)$ [N]: force generated by aponeurosis.
 - Model dependent variables: there are not such kind of parameters.

- Model independent parameters: there are not such kind of parameters.
- Model dependent parameters:
 - * l_A^{slack} [m]: slack length of aponeurosis.
 - * C_A [N/m²]: force-length coefficient. It means the force that is exerted when difference between the length of aponeurosis and the resting length of aponeurosis is one unit.
 - * V_A [Ns/m]: force-velocity coefficient.
- Model independent computed parameters: there are not such kind of parameters.
- Model dependent computed parameters: there are not such kind of parameters.

2.3.2 Value of parameters

This part gives the value of parameters if they are known with notation of this reference. The *GNrat* means that the data valid the gastrocnemius muscle of rat.

Parameter	Value	Source
<i>Sub-level of muscle</i>		
U_M^{th}	unknown, dep. on m.	[8]
r_M	dep. on m.	[8]
d_M^{dist}	dep. on m.	[8]
d_M^{prox}	dep. on m.	[8]
A	dep. on m.	
<i>Sub-level of tendon</i>		
D_T	dep. on m. 0.8-1.5-2GPa, (estimation: 10 ⁵)	[8]
C_T	unknown?, dep. on m., (estimation: 10 ⁴)	
l_T^{slack}	dep. on m.	
<i>Sublevel of tendon</i>		
C_A	0.16-0.38 N/mm ² <i>GNrat</i>	[40]
l_A^{slack}	19.8 mm <i>GNrat</i>	[40]
V_A	unknown?, dep. on m., (estimation: 10 ⁴)	

2.3.3 Analysis of degree of freedom

We investigate the degree of freedom of sub-levels separately.

- Sub-level of muscle: there are 11 variables or parameters that must be defined in the sub-level of muscle. There are 11 equations (2.26),(2.34)-(2.50) for define these variables and parameters. So the degree of freedom of sub-level of muscle is 0.
- Sub-level of tendon: there are 4 variables or parameters that must be defined in the sub-level of tendon. There are 4 equations (2.30),(2.31), (2.53), (2.54) for defining these variables and parameters. So the degree of freedom of sub-level of tendon is 0.
- Sub-level of aponeurosis: there are 3 variables or parameters that must be defined in the sub-level of aponeurosis. There are 3 equations (2.33), (2.32), (2.55) for defining these variables and parameters. So the degree of freedom of sub-level of aponeurosis is 0.

2.3.4 Analysis of the differential index of DAE

There are both differential and algebraic equations at the level of muscle. The structure matrix of the DAE model is presented in the tables below. We note that the variable or parameter in the () bracket means that this variable or parameter is defined in other level and not the currently investigated level. So this variable must be the one of the input of currently investigated level. We also note, that the constant parameters of this level are not in the table and sign \times means that the current variable, parameter is in the current equation while \otimes means that the current equation defines the current variable, parameter.

The structure matrix will be given at each level separately.

- Sub-level of muscle

	$l_{M+T}(t)$	$v_{M+T}(t)$	$l_M(t)$	$v_M(t)$	(l_A)	(v_A)	$\theta_{penn}(t)$	$\beta_{AM}(t)$	$\alpha_{FM}(t)$	$l_F(t)$	$v_F(t)$
(2.26)	×	⊗									
(2.34)			×	×	×	×	×			⊗	
(2.35)			×	×	×		×			×	⊗
(2.36)											
(2.37)											
(2.38)							×	×			
(2.40)			×				×	⊗		×	
(2.41)			(×)		(×)		×	×	⊗		
(2.42)											
(2.43)	⊗										
(2.44)	⊗										
(2.45)	(×)	⊗									
(2.47)	(×)	⊗									
(2.49)	×		⊗								
(2.50)		×		⊗							
(2.51)			×		×		⊗				
(2.52)			×		×		×				

	$f_F(t)$	$F_F^*(t)$	$F_M(t)$	$PCSA_M$	A	f_F^{min}	(f_F^{max})	$(U(t))$	$(F_F(t))$
(2.26)									
(2.34)									
(2.35)									
(2.36)	⊗			×		×	×	×	
(2.37)		⊗							×
(2.38)		×	⊗						
(2.40)									
(2.41)									
(2.42)				⊗					
(2.43)									
(2.44)									
(2.45)									
(2.47)									
(2.49)									
(2.50)									
(2.51)					×				
(2.52)					(⊗)				

	$(\alpha(t))$	$(\omega(t))$	$(l_T(t))$	$(v_T(t))$	$(PCSA_F)$
(2.26)					
(2.34)					
(2.35)					
(2.36)					×
(2.37)					
(2.38)					
(2.40)					
(2.41)					
(2.42)					×
(2.43)	×				
(2.44)	×				
(2.45)	×	×			
(2.47)	×	×			
(2.49)			×		
(2.50)				×	
(2.51)					
(2.52)					

Level of limb (L)
 Computes the acceleration of joint angles from the torques of muscles.

Variables	Parameters	Computed parameters
Model independent	Model independent	Model independent
$\alpha(t)$ [rad]	l [m]	—
$\omega(t)$ [rad/s]	m [kg]	
$\alpha^s(t)$ [rad]	g [m/s ²]	
$\omega^s(t)$ [rad/s]	\mathbf{r}^1 [m]	
$M_L(t)$ [Nm]	\mathbf{r}^2 [m]	
$\varphi(t)$ [rad]	Θ [kgm ²]	Model dependent
$\mathbf{F}_L(t)$ [N]	Model dependent	—
$\mathbf{a}(t)$ [m/s ²]	—	
$\mathbf{v}(t)$ [m/s]		
$\mathbf{s}(t)$ [m]		
$\mathbf{F}_{load}(t)$ [N]		
$M_{load}(t)$ [Nm]		
Model dependent		
—		

Figure 2.9: Structure of level of limb. Meaning of variables and parameters are in the paragraph **Variables and parameters**

- Sub-level of tendon

	l_T	v_T	(F_M)	F_T	M_M	(r_M)
(2.30)	⊗	×		×		
(2.31)	×	⊗				
(2.53)			×	⊗		
(2.54)				×	⊗	×

- Sub-level of aponeurosis

	l_A	v_A	F_A	(θ_{penn})	(F_F^*)
(2.33)	⊗	×			
(2.32)	×	⊗	×		
(2.55)			⊗	×	×

2.4 Level of limb

The level of limb contains the dynamic description of segments and joints. This level transforms the torques of muscles into joint rotations i.e into a real movement.

First the model equations will be constructed in the general case. We suppose that there are n pieces of segments and joints, i.e. $k = 1 \dots n$.

The structure of level of limb can be seen in Fig.2.9.

2.4.1 Model equations in original form

These equation are in the form of a set of differential and algebraic equation (DAE).

The differential equations of level of limb:

- Connection between the sum of joint angles and the sum of joint velocities

$$\frac{d\alpha_k^s(t)}{dt} = \omega_k^s(t) \tag{2.56}$$

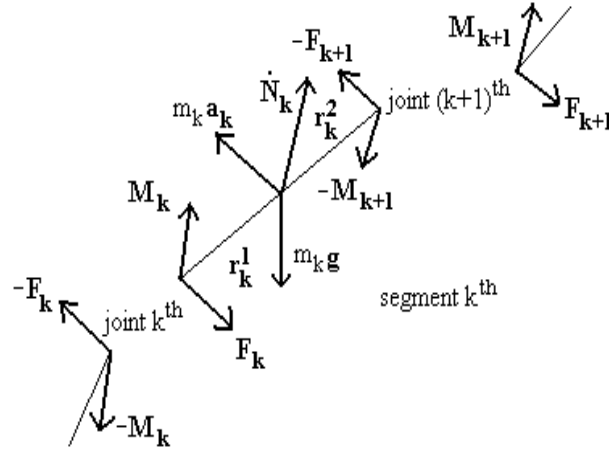


Figure 2.10: One segment with forces and torques.

- Differential equation of sum of joint velocities [47]

$$\frac{d\omega_k^s(t)}{dt} = \frac{1}{\theta_k} [M_{L,k}(t) - M_{L,k+1}(t) + |\mathbf{r}_k^1 \times \mathbf{F}_{L,k}(t)| - |\mathbf{r}_k^2 \times \mathbf{F}_{L,k+1}(t)|] \quad (2.57)$$

if $k = 1 \dots n - 1$ and

$$\frac{d\omega_n^s(t)}{dt} = \frac{1}{\theta_n} [M_{L,n}(t) - M_{load}(t) + |\mathbf{r}_n^1 \times \mathbf{F}_{L,n}(t)| - |\mathbf{r}_n^2 \times \mathbf{F}_{load}(t)|] \quad (2.58)$$

if $k = n$. In fig2.10 a segment and the its effected forces and torques are shown.

- Definition of segment velocities

$$\mathbf{v}_k(t) = \frac{d\mathbf{s}_k(t)}{dt} \quad (2.59)$$

- Definition of segment acceleration

$$\mathbf{a}_k(t) = \frac{d\mathbf{v}_k(t)}{dt} \quad (2.60)$$

The algebraic equations of the level of limb:

- Interface with the level of muscle

$$M_{L,k}(t) = \sum_{j \in k} M_{M,j}(t) \quad (2.61)$$

where $j \in k$ means that muscle j rotates the joint k .

- Define the sum of joint angles

$$\alpha_k^s(t) = \sum_{p=1}^k \alpha_p(t) \quad (2.62)$$

- Computing of interaction forces [47].

$$0 = \mathbf{F}_{L,k} - \mathbf{F}_{L,k+1} - m_k \mathbf{a}_k + m_k \mathbf{g} \quad (2.63)$$

if $k = 1 \dots n - 1$, and

$$0 = \mathbf{F}_{L,n} - \mathbf{F}_{load} - m_n \mathbf{a}_n + m_n \mathbf{g} \quad (2.64)$$

if $k = n$.

- Coordinates of center of mass of segment [46], [23].

$$\mathbf{s}_k(t) = \begin{bmatrix} \sum_{p=1}^{k-1} l_p \cos(\alpha_p^s(t)) + l_{COM,k} \cos(\alpha_k^s(t)) + x_0 \\ \sum_{p=1}^{k-1} l_p \sin(\alpha_p^s(t)) + l_{COM,k} \sin(\alpha_k^s(t)) + y_0 \end{bmatrix} \quad (2.65)$$

Variables and parameters of the level of limb are

- Model independent variables

- $\alpha^s(t)$ [rad]: the angle between the horizontal line and the line of given segment. It is the sum of the joint angles from the first joint to the given joint i.e.

$$\alpha_k^s(t) = \sum_{p=1}^k \alpha_p(t)$$

where $\alpha(t)$ [rad] is the joint angle of given joint.

- $\omega^s(t)$ [rad/s] is the time derivative of $\alpha^s(t)$, i.e. the angular velocity of the given segment.
- $\mathbf{F}_{L,k}$ [N,N] is the interaction force between segment $k - 1$ and k .
- $\mathbf{s}(t)$ [m,m] is the coordinate of the center of mass of given segment.
- $\mathbf{v}(t)$ [m/s,m/s] is the velocity of the center of mass of given segment.
- $M_L(t)$ [Nm] is the muscle torque in the given joint. It is a **known** scalar function of time. It is the input of level of limb, the generator of movement pattern.
- $M_{load}(t)$ [Nm]: external load torque. This torque is exerted by the environment to the tip of the limb. It is a **known** scalar function of time.
- $\mathbf{F}_{load}(t)$ [N,N]: external load force. This force is exerted by the environment to the tip of the limb. It is a **known** vectorial function of time.

- Model dependent variables: none

- Model independent parameters

- m [kg] is the mass of the given segment.
- l [m] is the length of the given segment.
- $l_{COM,k}$ [m] is the distance between the joint k and center of mass of segment k .
- θ [kgm²] is the moment of inertia of the given segment.
- \mathbf{g} [m/s²,m/s²]: vector of gravitational acceleration.
- \mathbf{r}^1 [m,m]: vector pointing from the center of mass of the given segment to segment's proximal joints.
- \mathbf{r}^2 [m,m]: vector pointing from the center of mass of the given segment to segment's distal joints.
- α_0 [rad]: initial value of the given joint angle.
- ω_0 [rad/s]: initial value of the velocity of given joint.
- β_0 [rad/s²]: initial value of the acceleration of given joint.
- (x_0, y_0) [m,m]: coordinate of the first joint.

- Model dependent parameters: none

- Model independent computed parameters: none

- Model dependent computed parameters: none

2.4.2 Value of parameters

This part gives the value of parameters that can be found in the literature with a pointer to their reference.

Parameter	Value	Source
m	dep. on m.	[8], [47]
l	dep. on m.	[8], [47]
l_{COM}	dep. on m.	[8], [47]
θ	dep. on m.	[8], [47]
g	9.81 m/s ² on Earth	[8], [47]
\mathbf{r}^1	dep. on m.	[8], [47]
\mathbf{r}^2	dep. on m.	[8], [47]
(x_0, y_0)	arbitrary	give by user

2.4.3 Analysis of degree of freedom

Having completed the analysis of degree of freedom, the result was that the degree of freedom of this level of the limb model is 0, i.e. the number of equations and the number of variables are the same. There are 10 variables and 10 equations for each joint and segment. The variables are: $\alpha_k^s(t)$, $\omega_k^s(t)$, $\mathbf{F}_{L,k}(t)$, $\mathbf{s}_k(t)$, $\mathbf{v}_k(t)$ and $\mathbf{a}_k(t)$ where the last four are vector, so they have got two elements. The equations are (2.57), (2.56), (2.63), (2.60) (2.59) and (2.65) where the last four equations are vector equations, so they have to have two components.

2.4.4 Investigation of the differential index of DAE

The structure matrix can be seen in the table below. We note that the variable or parameter in the () bracket means that this variable or parameter is defined in other level and not the currently investigated level. So this variable must be the one of the input of currently investigated level. We also note, that the constant parameters of this level are not in the table and sign \times means that the current variable, parameter is in the current equation while \otimes means that the current equation defines the current variable or parameter, respectively.

	$\alpha^s(t)$	$\omega^s(t)$	$s(t)$	$v(t)$		$f_L(t)$	$a(t)$	$M_L(t)$	$(M_F(t))$	$\alpha(t)$
(2.56)	\otimes	\times								
(2.57)		\otimes				\times		\times		
(2.59)			\times	\otimes						
(2.60)				\times			\otimes			
(2.61)								\otimes	\times	
(2.62)	\times									\otimes
(2.63)						\otimes	\times			
(2.65)	\times		\otimes							

As it can be seen, the first four variables are the differential variables and the first four equations are the differential equations. The last four variables and equations are the algebraic variables and equations, respectively.

In the row of equation (2.65) there is no algebraic algebraic variable. Thus the **differential index of this DAE system is greater than 1**. The reason for this is the over-determination of the differential variables $\alpha_k^s(t)$ or $\omega_k^s(t)$. It means that $\alpha_k^s(t)$ is determined by Eqn.(2.57) while it must also satisfy Eqn.(2.65).

Chapter 3

Model solution and verification

A multilevel hierarchical model of a limb system is derived and presented in Chapter 2. The solvability analysis has been performed separately for each level assuming that the interface-variables are given constants for the investigated sub-model.

This chapter deals with the models solution including the transformation of the model into a solvable form and the verification of the model against engineering expectations.

3.1 Model transformation of the sub-model on the level of limb

During the solvability analysis it has turned out in section 2.4.4, that the only problematic level is the level of limb, where the resulting model is a higher index one. In order to improve the situation, Eqn.(2.65) is substituted into Eqn.(2.59) and the resulting equation is substituted into Eqn.(2.60). Furthermore, the result is substituted into Eqn.(2.63) and then Eqn.(2.57). During this computation we use that

$$|\mathbf{r}_{\mathbf{k}}^1 \times \mathbf{F}_{\mathbf{L},\mathbf{k}}| = r_{k,x}^1 F_{L,k,y} - r_{k,y}^1 F_{L,k,x}$$

where x and y mean the x and y coordinate of the variable, respectively.

As a result of this computation we get that

$$\begin{aligned}
\theta_k \frac{d\omega_k^s(t)}{dt} &= M_{L,k}(t) - M_{L,k+1}(t) - \\
&- r_{k,x}^1 m_k \left[\sum_{p=1}^{k-1} l_p (\sin \alpha_p^s(t)) (\omega_p^s(t))^2 \right] - r_{k,x}^1 m_k l_{COM,k} (\sin \alpha_k^s(t)) (\omega_k^s(t))^2 - \\
&- [r_{k,x}^1 - r_{k,x}^2] \sum_{l=k+1}^n \left(m_l \left[\sum_{p=1}^{l-1} l_p (\sin \alpha_p^s(t)) (\omega_p^s(t))^2 \right] \right) - \\
&- [r_{k,x}^1 - r_{k,x}^2] \sum_{l=k+1}^n \left(m_l l_{COM,l} (\sin \alpha_l^s(t)) (\omega_l^s(t))^2 \right) + \\
&+ r_{k,x}^1 m_k \left[\sum_{p=1}^{k-1} l_p (\cos \alpha_p^s(t)) \dot{\omega}_p^s(t) \right] + r_{k,x}^1 m_k l_{COM,k} (\cos \alpha_k^s(t)) \dot{\omega}_k^s(t) + \\
&+ [r_{k,x}^1 - r_{k,x}^2] \sum_{l=k+1}^n \left(m_l \left[\sum_{p=1}^{l-1} l_p (\cos \alpha_p^s(t)) \dot{\omega}_p^s(t) \right] \right) + \\
&+ [r_{k,x}^1 - r_{k,x}^2] \sum_{l=k+1}^n \left(m_l l_{COM,l} (\cos \alpha_l^s(t)) \dot{\omega}_l^s(t) \right) + \\
&+ r_{k,y}^1 m_k \left[\sum_{p=1}^{k-1} l_p (\cos \alpha_p^s(t)) (\omega_p^s(t))^2 \right] + r_{k,y}^1 m_k l_{COM,k} (\cos \alpha_k^s(t)) (\omega_k^s(t))^2 + \\
&+ [r_{k,y}^1 - r_{k,y}^2] \sum_{l=k+1}^n \left(m_l \left[\sum_{p=1}^{l-1} l_p (\cos \alpha_p^s(t)) (\omega_p^s(t))^2 \right] \right) + \\
&+ [r_{k,y}^1 - r_{k,y}^2] \sum_{l=k+1}^n \left(m_l l_{COM,l} (\cos \alpha_l^s(t)) (\omega_l^s(t))^2 \right) + \\
&+ r_{k,y}^1 m_k \left[\sum_{p=1}^{k-1} l_p (\sin \alpha_p^s(t)) \dot{\omega}_p^s(t) \right] + r_{k,y}^1 m_k l_{COM,k} (\sin \alpha_k^s(t)) \dot{\omega}_k^s(t) + \\
&+ [r_{k,y}^1 - r_{k,y}^2] \sum_{l=k+1}^n \left(m_l \left[\sum_{p=1}^{l-1} l_p (\sin \alpha_p^s(t)) \dot{\omega}_p^s(t) \right] \right) + \\
&+ [r_{k,y}^1 - r_{k,y}^2] \sum_{l=k+1}^n \left(m_l l_{COM,l} (\sin \alpha_l^s(t)) \dot{\omega}_l^s(t) \right) - \\
&- m_k [r_{k,x}^1 g_y - r_{k,y}^1 g_x] - ([r_{k,x}^1 - r_{k,x}^2] g_y - [r_{k,y}^1 - r_{k,y}^2] g_x) \sum_{l=k+1}^n m_l + \\
&+ (r_{k,x}^1 - r_{k,x}^2) F_{load,y} - (r_{k,y}^1 - r_{k,y}^2) F_{load,x}
\end{aligned}$$

where $k = 1 \dots n-1$. If $k = n$, then we get the same result, but we have to omit terms containing sum from index $k+1$. During the computation we use that

$$\begin{aligned}
\sum_{p=1}^l \left(\left[\sum_{r=p}^{l-1} l_r (\sin \alpha_r^s(t)) \omega_r^s(t) \right] \omega_p(t) \right) &= \sum_{p=1}^{l-1} \left(\left[\sum_{r=p}^{l-1} l_r (\sin \alpha_r^s(t)) \omega_r^s(t) \right] \omega_p(t) \right) = \\
&= \sum_{p=1}^{l-1} l_p (\sin \alpha_p^s(t)) (\omega_p^s(t))^2
\end{aligned}$$

and

$$\begin{aligned} \sum_{p=1}^k \left(\left[\sum_{r=p}^{k-1} l_r \sin \alpha_r^s(t) \right] \dot{\omega}_p(t) \right) &= \sum_{p=1}^{k-1} \left(\left[\sum_{r=p}^{k-1} l_r \sin \alpha_r^s(t) \right] \dot{\omega}_p(t) \right) = \\ &= \sum_{p=1}^{k-1} l_p (\sin \alpha_p^s(t)) \dot{\omega}_p^s(t) \end{aligned}$$

We can perform a similar computation for the terms containing cosine function. Then we can notice that that there is a growing number of derivative terms in each equation. We can group these additional terms by using the expression

$$\begin{aligned} &\sum_{l=k+1}^n \left(m_l \left[\sum_{p=1}^{l-1} l_p (\cos \alpha_p^s(t)) \dot{\omega}_p^s(t) \right] \right) = \\ &= \sum_{p=1}^k \dot{\omega}_p^s(t) \left[l_p (\cos \alpha_p^s(t)) \sum_{r=k+1}^n m_r \right] + \sum_{p=k+1}^{n-1} \dot{\omega}_p^s(t) \left[l_p (\cos \alpha_p^s(t)) \sum_{r=p+1}^n m_r \right] \end{aligned}$$

to obtain for $k = 1 \dots n - 1$

$$\begin{aligned} &\sum_{p=1}^n a_{k,p}(\alpha_1^s(t), \dots, \alpha_n^s(t)) \dot{\omega}_p^s(t) = \\ &= M_{L,k}(t) - M_{L,k+1}(t) + F_k(\alpha_1^s, \dots, \alpha_n^s(t), \omega_1^s(t), \dots, \omega_n^s(t)) + G_k \end{aligned} \quad (3.1)$$

where the value of $a_{k,p}$ depends on the the value of p :

$$\begin{aligned} &a_{k,k}(\alpha_1^s(t), \dots, \alpha_n^s(t)) = \\ &= \theta_k - l_k \left([r_{k,x}^1 - r_{k,x}^2] \cos \alpha_k^s(t) + [r_{k,y}^1 - r_{k,y}^2] \sin \alpha_k^s(t) \right) \left(\sum_{r=k+1}^n m_r \right) - \\ &\quad - m_k l_{COM,k} \left(r_{k,x}^1 \cos \alpha_k^s(t) + r_{k,y}^1 \sin \alpha_k^s(t) \right) \end{aligned} \quad (3.2)$$

and

$$\begin{aligned} &a_{k,p}(\alpha_1^s(t), \dots, \alpha_n^s(t)) = \\ &= -l_p \left([r_{k,x}^1 - r_{k,x}^2] \cos \alpha_p^s(t) + [r_{k,y}^1 - r_{k,y}^2] \sin \alpha_p^s(t) \right) \left(\sum_{r=k+1}^n m_r \right) - \\ &\quad - l_p m_k \left(r_{k,x}^1 \cos \alpha_p^s(t) + r_{k,y}^1 \sin \alpha_p^s(t) \right) \end{aligned} \quad (3.3)$$

if $p < k$, i.e. $p = 1, \dots, k - 1$ and

$$\begin{aligned} &a_{k,p}(\alpha_1^s(t), \dots, \alpha_n^s(t)) = \\ &= -l_p \left([r_{k,x}^1 - r_{k,x}^2] \cos \alpha_p^s(t) + [r_{k,y}^1 - r_{k,y}^2] \sin \alpha_p^s(t) \right) \left(\sum_{r=p+1}^n m_r \right) - \\ &\quad - l_{COM,p} m_p \left([r_{k,x}^1 - r_{k,x}^2] \cos \alpha_p^s(t) + [r_{k,y}^1 - r_{k,y}^2] \sin \alpha_p^s(t) \right) \end{aligned} \quad (3.4)$$

if $k < p < n$, i.e. $p = k + 1, \dots, n - 1$ and

$$\begin{aligned} &a_{k,n}(\alpha_1^s(t), \dots, \alpha_n^s(t)) = \\ &= -m_n l_{COM,n} \left([r_{k,x}^1 - r_{k,x}^2] \cos \alpha_n^s(t) + [r_{k,y}^1 - r_{k,y}^2] \sin \alpha_n^s(t) \right) \end{aligned} \quad (3.5)$$

if $p = n$ and

$$\begin{aligned}
F_k(\alpha_1^s(t), \dots, \alpha_n^s(t), \omega_1^s(t), \dots, \omega_n^s(t)) &= -r_{k,x}^1 m_k \left[\sum_{p=1}^{k-1} l_p (\sin \alpha_p^s(t)) (\omega_p^s(t))^2 \right] - \\
&\quad - r_{k,x}^1 m_k l_{COM,k} (\sin \alpha_k^s(t)) (\omega_k^s(t))^2 - \\
&\quad - \left[r_{k,x}^1 - r_{k,x}^2 \right] \sum_{l=k+1}^n \left(m_l \left[\sum_{p=1}^{l-1} l_p (\sin \alpha_p^s(t)) (\omega_p^s(t))^2 \right] \right) - \\
&\quad - \left[r_{k,x}^1 - r_{k,x}^2 \right] \sum_{l=k+1}^n \left(m_l l_{COM,l} (\sin \alpha_l^s(t)) (\omega_l^s(t))^2 \right) + \\
&\quad + r_{k,y}^1 m_k \left[\sum_{p=1}^{k-1} l_p (\cos \alpha_p^s(t)) (\omega_p^s(t))^2 \right] + \\
&\quad + r_{k,y}^1 m_k l_{COM,k} (\cos \alpha_k^s(t)) (\omega_k^s(t))^2 + \\
&\quad + \left[r_{k,y}^1 - r_{k,y}^2 \right] \sum_{l=k+1}^n \left(m_l \left[\sum_{p=1}^{l-1} l_p (\cos \alpha_p^s(t)) (\omega_p^s(t))^2 \right] \right) + \\
&\quad + \left[r_{k,y}^1 - r_{k,y}^2 \right] \sum_{l=k+1}^n \left(m_l l_{COM,l} (\cos \alpha_l^s(t)) (\omega_l^s(t))^2 \right) + \\
&\quad + (r_{k,x}^1 - r_{k,x}^2) F_{load,y} - (r_{k,y}^1 - r_{k,y}^2) F_{load,x} \tag{3.6}
\end{aligned}$$

and the gravitational term is

$$G_k = -m_k [r_{k,x}^1 g_y - r_{k,y}^1 g_x] - ([r_{k,x}^1 - r_{k,x}^2] g_y - [r_{k,y}^1 - r_{k,y}^2] g_x) \sum_{l=k+1}^n m_l \tag{3.7}$$

In eqn.(3.1)-(3.7) the value of k is $k = 1 \dots n - 1$. If $k = n$ then we get the same result but the tags containing index $k + 1$ must be neglected (they are zeros) and the loading tag must be added. So in this case the equations are

$$\begin{aligned}
&\sum_{p=1}^n a_{n,p}(\alpha_1^s(t), \dots, \alpha_n^s(t)) \dot{\omega}_p^s(t) = \\
&= M_{L,n}(t) - M_{load}(t) + F_n(\alpha_1^s, \dots, \alpha_n^s(t), \omega_1^s(t), \dots, \omega_n^s(t)) + G_n
\end{aligned}$$

where

$$\begin{aligned}
a_{n,n}(\alpha_1^s(t), \dots, \alpha_n^s(t)) &= \\
&= \theta_n - m_n l_{COM,n} [r_{n,x}^1 \cos \alpha_n^s(t) + r_{n,y}^1 \sin \alpha_n^s(t)]
\end{aligned}$$

if $p = n$ and

$$\begin{aligned}
a_{n,p}(\alpha_1^s(t), \dots, \alpha_n^s(t)) &= \\
&= -m_n l_p [r_{n,x}^1 \cos \alpha_p^s(t) + r_{n,y}^1 \sin \alpha_p^s(t)]
\end{aligned}$$

where $p = 1 \dots n - 1$ and

$$\begin{aligned}
F_n(\alpha_1^s(t), \dots, \alpha_n^s(t), \omega_1^s(t), \dots, \omega_n^s(t)) &= \\
&= -m_n \sum_{p=1}^{n-1} l_p (\omega_p^s(t))^2 [r_{n,x}^1 \sin \alpha_p^s(t) + r_{n,y}^1 \cos \alpha_p^s(t)] - \\
&\quad - m_n l_{COM,n} (\omega_n^s(t))^2 [r_{n,x}^1 \sin \alpha_n^s(t) + r_{n,y}^1 \cos \alpha_n^s(t)] - \\
&\quad + (r_{n,x}^1 - r_{n,x}^2) F_{load,y}(t) - (r_{n,y}^1 - r_{n,y}^2) F_{load,x}(t)
\end{aligned}$$

and the gravitational term

$$G_n = -m_n [r_{n,x}^1 g_y - r_{n,y}^1 g_x]$$

3.1.1 Solvability analysis of the transformed model

Let's analyze this solution. According to the definition of vector \mathbf{r}_k^1 and \mathbf{r}_k^2 there are parallel with the line of the segment k in 2D. But while vector \mathbf{r}_k^1 shows from center of mass of segment k to the joint k the vector \mathbf{r}_k^2 shows from center of mass of segment k to the joint $k+1$ or to the tip of the limb if $k=n$. It means that

$$|\mathbf{r}_k^1| = r_k^1 = l_{COM,k}$$

and

$$|\mathbf{r}_k^1 - \mathbf{r}_k^2| = l_k$$

where $k = 1 \dots n$.

Scalar product is defined by expression $\langle \mathbf{a}, \mathbf{b} \rangle = \sum_{p=1}^m a_p b_p$ where \mathbf{a} and \mathbf{b} is element of $R^{m \times 1}$ and $\mathbf{a} = [a_1 \dots a_m]$ and $\mathbf{b} = [b_1 \dots b_m]$. According to this definition you can see that

$$r_{k,x}^1 \cos \alpha_k^s(t) + r_{k,y}^1 \sin \alpha_k^s(t) = \langle \mathbf{r}_k^1, [\cos \alpha_k^s(t), \sin \alpha_k^s(t)] \rangle$$

where $[\cos \alpha_k^s(t), \sin \alpha_k^s(t)]$ is a direction vector of segment k in current moment. According to the property of scalar product and property of 2D limb model:

$$r_{k,x}^1 \cos \alpha_k^s(t) + r_{k,y}^1 \sin \alpha_k^s(t) = -l_{COM,k}$$

Similarly

$$[r_{k,x}^1 - r_{k,x}^2] \cos \alpha_k^s(t) + [r_{k,y}^1 - r_{k,y}^2] \sin \alpha_k^s(t) = -l_k$$

These expressions make possible to us to simplify the expression $a_{k,k}$. According to them

$$a_{k,k} = \theta_k + l_k^2 \left(\sum_{r=k+1}^n m_r \right) + m_k l_{COM,k}^2 \quad (3.8)$$

if $k = 1 \dots n-1$ and

$$a_{n,n} = \theta_n + m_n l_{COM,n}^2 \quad (3.9)$$

if $k = n$. We can establish that $a_{k,k}$, $k = 1 \dots n$ are independent from the joint angles.

Since the definition of sum of joint velocity is known from (2.56) we note that (3.1) differential equations with (2.56) differential equations ($k = 1 \dots n$) establish a system of differential equations where the differential variables are $\alpha_1^s(t), \dots, \alpha_n^s(t), \omega_1^s(t), \dots, \omega_n^s(t)$ and the differential equations are

$$\frac{d\alpha^s}{dt} = \omega^s \quad (3.10)$$

$$\frac{d\omega^s}{dt} = \mathbf{A}(\alpha^s)^{-1} (\mathbf{M} + \mathbf{F}(\alpha^s, \omega^s) + \mathbf{G}) \quad (3.11)$$

if the inverse of matrix \mathbf{A} exists and where

$$\alpha^s = [\alpha_1^s \dots \alpha_n^s]^T \in R^{n \times 1} \quad (3.12)$$

$$\omega^s = [\omega_1^s \dots \omega_n^s]^T \in R^{n \times 1} \quad (3.13)$$

$$\mathbf{A} = (a_{k,p})_{k,p=1}^n \in R^{n \times n} \quad (3.14)$$

$$\mathbf{M} = [M_{L,1} - M_{L,2} \dots M_{L,n-1} - M_{L,n}, M_{L,n} - M_{load}]^T \in R^{n \times 1} \quad (3.15)$$

$$\mathbf{F} = [F_1 \dots F_n]^T \in R^{n \times 1} \quad (3.16)$$

$$\mathbf{G} = [G_1 \dots G_n]^T \in R^{n \times 1} \quad (3.17)$$

and $a_{k,p}$ are defined according to (3.8), (3.3), (3.4) and (3.5) while F_k and G_k are defined in (3.6) and (3.7), respectively. According to these definition \mathbf{A} depends on the α_k^s , $k = 1 \dots n$ while vector \mathbf{F} depends on the α_k^s and ω_k^s , $k = 1 \dots n$ and vector \mathbf{G} independents from the differential variables. Exactly, since the direction of vector \mathbf{r}_k^1 and vector \mathbf{r}_k^2 depend on the direction of the segment k^{th} , so the vector \mathbf{G} depends on the sum of joint angles indirectly. The matrix \mathbf{M} is the input of the limb, it contains the torques of joints.

As we mentioned above to solve easily the new model equations (3.10) and (3.11) the inverse of matrix \mathbf{A} must exist. According to the (3.8) and (3.9) we know that there are positive values in the diagonal elements of matrix \mathbf{A} . Let's investigate the other elements of matrix \mathbf{A} . We use the following inequalities for this estimation what are the consequences of property of scalar product:

$$-l_{COM,k} \leq r_{k,x}^1 \cos \alpha_p^s(t) + r_{k,y}^1 \sin \alpha_p^s(t) \leq l_{COM,k}$$

and

$$-l_k \leq [r_{k,x}^1 - r_{k,x}^2] \cos \alpha_p^s(t) + [r_{k,y}^1 - r_{k,y}^2] \sin \alpha_p^s(t) \leq l_k$$

where $p \neq k$. So the estimations are:

$$|a_{k,p}| \leq \begin{cases} l_p l_k \left(\sum_{r=k+1}^n m_r \right) + l_p l_{COM,k} m_k & \text{if } p = 1 \dots k-1 \text{ and } k \neq n \\ l_p l_k \left(\sum_{r=k+1}^n m_r \right) + l_k l_{COM,p} m_p & \text{if } p = k+1 \dots n-1 \text{ and } k \neq n \\ m_n l_{COM,n} l_k & \text{if } p = n \text{ and } k \neq n \end{cases} \quad (3.18)$$

and if $k = n$

$$|a_{n,p}| \leq l_p l_{COM,n} m_n \quad (3.19)$$

where $p = 1 \dots n-1$. According to (3.18) and (3.19) the non-diagonal element of matrix \mathbf{A} should be positive and negative while diagonal elements are always positive. It means that in general case the matrix \mathbf{A} is invertible, but may be some joint angles configuration where matrix \mathbf{A} become singular.

Investigate the rank of matrix \mathbf{A} with Maple, we get that the matrix \mathbf{A} is full rank matrix, i.e. invertible. Matrix \mathbf{A} plays role of inertia matrix.

There is no problem with the initial condition in the equations (3.10) and (3.11). The problem of initial condition existed in the original form of equations because the $\alpha^s(\mathbf{t})$ was defined by equation (2.56) while it must have been satisfied equation (2.65) where the coordinates of segments were given. It means that we modelled the limb in two spaces: in space of joints and in 2D space. The connection between these two space were defined by equation (2.65). But in the new form of equations of level of limb only the space of joint plays role, because we transformed the 2D space into the space of joint via equation (2.65). So the initial values should be defined uniquely in this new form of equations.

3.1.2 Computational steps on the level of limb

Suppose that the current value of sum of joint angles $\alpha_k^s(t)$, $k = 1 \dots n$, sum of joint velocities $\omega_k^s(t)$, $k = 1 \dots n$, current length of tendons $l_{T,j}(t)$, current length of aponeurosis $l_{A,j}(t)$, their current contraction velocities $v_{T,j}(t)$, $v_{A,j}(t)$ and the area of the muscles A_j are known.

We note that the A_j was chosen as a known parameter because it is constant. But the value of $\theta_{penn,j}$ must be known to do the computation. However the values of $\theta_{penn,j}$ can be computed from the area of the muscle, the initial length of aponeurosis and the initial length of muscle.

1. Level of limb computes the joint angles and the joint velocities from the sum of joint angles and the sum of the joint velocities. The level of limb gets the current input signals and forwards them together with the value of joint angles to the level of muscle, sub-level of muscle.
2. Sub-level of muscle determines the length of muscle-tendon complex $l_{M+T,j}(t)$ from the joint angles and the contraction velocity of muscle-tendon complex $v_{M+T}(t)$ from the joint velocities. Using the length of tendon $l_{T,j}(t)$ and contraction velocity of tendon $v_{T,j}(t)$ this sub-level computes the length of muscle $l_{M,j}(t)$ and the contraction velocity of the muscle $v_{M,j}(t)$. Then the length of fibers $l_{F,i}(t)$ and the contraction velocity of fiber $v_{F,i}(t)$ are computed where $i \in j$ from the $l_{A,j}(t)$, $\theta_{penn,j}(t)$, $l_{M,j}(t)$ and $l_{A,j}(t)$, $v_{A,j}(t)$, $\theta_{penn,j}(t)$, $l_{M,j}(t)$, $v_{M,j}(t)$ respectively. From length of fibers and length of muscle this sub-level determines the current value of $\beta_{AM,j}(t)$ and then the value $\alpha_{FM,j}(t)$ is computed from the value of $\beta_{AM,j}(t)$ and the pennate angle $\theta_{penn,j}(t)$. Then this sub-level computes the exciting frequency of each fiber from the input activation signals. The length of fiber $l_{F,i}$, contraction velocity of fiber $v_{F,i}$, and the exciting frequency of fiber $f_{F,i}$ are forwarded to the level of fiber.

3. The level of fiber computes length of sarcomere $l_{S,q}(t)$, the contraction velocity of sarcomere $v_{S,q}(t)$ and the exciting frequency of sarcomere $f_{S,q}(t)$ from the given value of $v_{F,i}$, $l_{F,i}$ and $f_{F,i}$ where $q \in i$. Then it determines the passive force F_{PE} and if necessary the value of *force-length of muscle* characteristic FL and value of *force-frequency* characteristic FF . The $l_{S,q}$, $v_{S,q}$ and $f_{S,q}$ are forwarded to the level of sarcomere.
4. Level of sarcomere computes the current exerted force of sarcomere $F_{S,q}(t)$ from the given values of $l_{S,q}$, $v_{S,q}$ and $f_{S,q}$. The $F_{S,q}(t)$ are forwarded to the level of fiber.
5. Level of fiber computes the current exerted force of fiber $F_{F,i}(t)$ from the given value of force of sarcomere $F_{S,q}(t)$ and the previously computed value of force-length FL , force frequency FF and passive force F_{PE} . The value of $F_{F,i}(t)$ are forwarded to the level of muscle, sub-level of muscle.
6. Level of muscle, sub-level of muscle computes the sum of force of fibers $F_{F,j}^*(t)$ and computes the force of muscle $F_{M,j}$ using the value of pennate angle. The $F_{M,j}$ forward its value together with other necessary values to the sub-level of tendon while the value of $F_{F,j}^*$ with the other necessary values are forwarded to the sub-level of aponeurosis.
 - Sub-level of tendon computes the force of tendon $F_{T,j}$ and then the contraction velocity of tendon $v_{T,j}$ from the $F_{T,j}$ and the length of the tendon from the $l_{T,j}$. Then the torque of muscle $M_{M,j}$ is computed from the $F_{T,j}$ and $r_{M,j}$. The $v_{T,j}$, $l_{T,j}$ and $M_{M,j}$ are forwarded to the sub-level of muscle.
 - Sub-level of aponeurosis computes the force of aponeurosis $F_{A,j}$ from the $F_{F,j}^*$, $\alpha_{FM,j}$ and $\beta_{AM,j}$. Then it computes contraction velocity of aponeurosis $v_{A,j}$ and then it computes the length of aponeurosis $l_{A,j}$. The $l_{A,j}$, $v_{A,j}$ and $F_{A,j}$ are forwarded to the sub-level of muscle.

Then the sub-level of muscle computes the derivative of pennate angle from the new value of $l_{F,j}$, $v_{F,j}$, $l_{A,j}$, $v_{A,j}$ and the value of pennate angle and then it computes the new value of pennate angle.

The sub-level of muscle forward the torque of muscle $M_{M,j}$ to the level of limb.

7. Level of limb integrates the torques exerted in the same joints and get the torque of joint $M_{L,k}$. Then solve the differential equation system of limb and determine the next value of sum of joint angles $\alpha_k^s(t)$ and sum of joint velocity $\omega_k^s(t)$. The $\alpha_k^s(t)$, $\omega_k^s(t)$ and the next value of activation signal is forwarded to the level of muscle, sub-level of muscle and the computation cycle starts again from the step 2.

3.2 The method of solving the DAE model

The above described hierarchical limb model is realized in MATLAB. The structure of the simulation program follows the structure of the model: each level of model is realized in a different *.m* file. To solve the dynamic equations on the level of limb the *ode15s* function is used. The matrix \mathbf{A} is realized as a mass matrix. For better and faster computation the Jacobian matrix is also computed and programmed. Data of each of the levels are stored in a suitable structure.

3.2.1 Model inputs and outputs

The main model input is the activation signal of each muscle. An activation signal is described by using the envelope of the EMG. There are also some other modifactor inputs: the force and torque of the environment effecting the tip of the limb. Using this functionality we can simulate movements when a person e.g lifts weights. To complete the simulation the user has to define the segments, muscles and initial position and orientation of the segments.

The output of the model is the movement pattern of the limb. Moreover the user also receives the value of characteristic variables of limb in time such as joint angles, joint velocities, lengths and contraction velocities of tendons, muscles, fibers, sarcomeres, exerted forces of sarcomeres, fibers, muscles etc.

3.2.2 The numerical method

The equations of level of limb are solved with *ode15s* that is applicable to both differential and DAE equations. The *ode15s* solver is a variable-order solver based on the numerical differentiation formulas (NDFs) [32]. Optionally it uses the backward differentiation formulas, BDFs, (also known as Gear's method). It is a multistep solver. After each successful integration step the current joint angles and joint velocities are given to the level of muscle. This level and level of fiber and sarcomere compute the force of sarcomere, force of fiber and finally the force of muscle. After that, the level of tendon computes the contraction velocity of tendon solving the corresponding differential equation with *ode45* that is a *Runge-Kutta 4* method [32]. To compute the dynamic behavior of aponeurosis the *ode45* function is used.

3.2.3 Initial values of the parameters

Initial values of the parameters are determined according to the information found in literature. In the case when there is no value of the current parameter in the literature we have used an estimated value. In the subsections of *Values of parameters* above these initial values and their source are found.

The initial values of variables are given by the user based on his/her measurement.

3.3 Model verification

Model verification is a standard step in the systematic way of model building we follow here. The aim of the model verification is to check that the model behaves in a reasonable way. It means that we excite the muscles with known activation signals and check that the model behaves as we expect. It is not the same as model validation where the model is checked against reality.

Another important aim of the model verification is to generate movement patterns that we can describe verbally. The most important property of the measurements to be used later for parameter estimation is that the input i.e. the activation signal, cannot be influenced directly during the measurement. It means that the activation signal is generated by the nervous system of the measured human being. We tell him/her what he/she has to do but we cannot influence the activation signal by using electrodes.

3.3.1 Verification test cases: a single joint limb

The verification has been performed step by step by using a top-down approach.

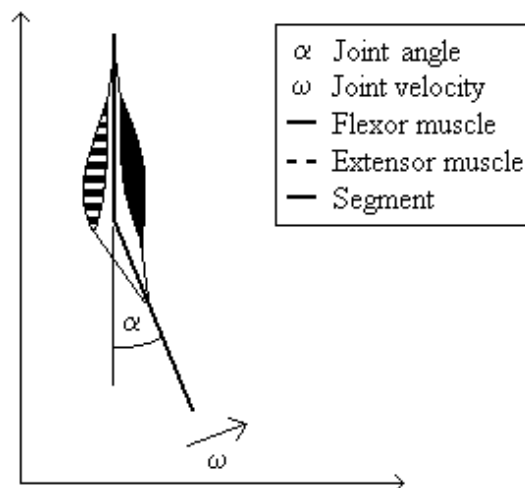


Figure 3.1: *The simplest limb with one joint. This limb is used in this section.*

The first step of the verification is the verification of the movement of a limb containing only one joint. First we verify the upper level of the model i.e. the level of limb, then level of muscle, level of fiber, level of sarcomere and finally the level of tendon (and aponeurosis). In the simplest case a limb contains one

joint, one flexor muscle and one extensor muscle. Both muscle contains only one fiber and one kind of sarcomere. This simplest limb has got two segment: the first is fixed and the second can rotate around the joint. Gravitation influences the movement of the limb. This simplest limb is shown in fig.3.1.

Verification of level of limb To verify the level of limb alone we assume that there are no muscles in the limb. It means that the movement of joint is influenced only by the inertia moments of segments, the gravitation and initial value of joint angle and joint velocity. We expect that the movement of the limb is the same as the movement of a pendulum. This kind of motion can be seen in fig. 3.2. In this case the initial joint angle is 30 [degree], initial joint velocity is 0 [rad/s], gravitational acceleration is 1.1 [m/s²]. As it is shown in the fig.3.2 the joint angle and the joint velocity is sinusoidal function of time, the frequency of motion is approximately 1/3 Hz.

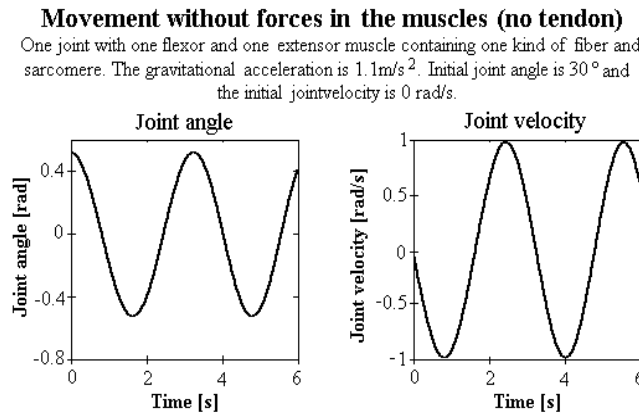


Figure 3.2: Behavior of the limb if there is no force in the muscles. Gravitational acceleration is 1.1 [m/s²]

To test the gravitational effect, a new simulation with 9.81 m/s² acceleration is created. We expected that the frequency of pendulum increases if the gravitational acceleration increases. The joint angle and joint velocity of limb is shown in fig.3.3. In this case the initial joint angle is 30 [degree], initial joint velocity is 0 [rad/s], as in the previous simulation. As it is shown in fig.3.3 the joint angle and the joint velocity is sinusoidal function of time, the frequency of motion is approximately 1 Hz. Comparing this frequency to the frequency of pendulum motion in lower gravitational field, the conclusion is that if the gravitational acceleration increases then the frequency of the pendulum motion also increases, as we expected.

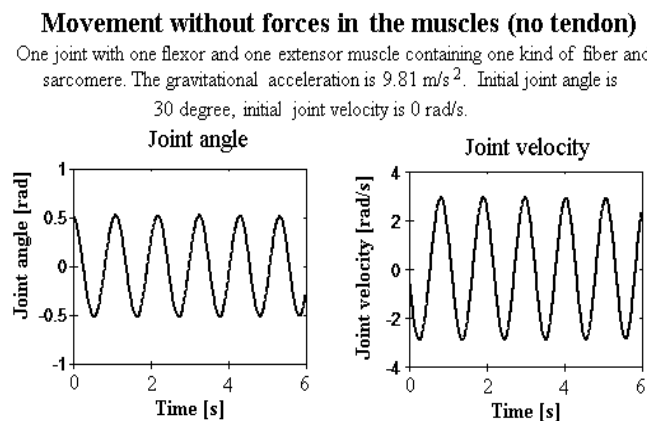


Figure 3.3: Behavior of the limb if there is no force in muscles. Gravitational acceleration is 9.81 [m/s²]

To test the behavior of limb in loaded case we create the same simulation but there is a 200 N load at vertical down direction, as if the subject holds a 20 kg weight. We expect that the frequency of the pendulum increases. The joint angle and joint velocity of limb is shown in fig.3.4. We use the same initial condition as

previously: Initial joint angle is 30 [degree], initial joint velocity is 0 [rad/s] and the gravitational acceleration is 9.81 [m/s²]. As it is shown in fig.3.4 the joint angle and the joint velocity is sinusoidal function of time, the frequency of motion is approximately 6 Hz. Comparing this frequency to the frequency of pendulum motion without load, the conclusion is that if the load increases then the frequency of the pendulum motion also increases, as we expected.

Movement of limb: no force in muscles, load, no tendon and no pennation

There is one joint with one flexor and one extensor muscle, but there is no force in the muscle.
 There is a 200 N load at vertical down direction in the tip of the limb.
 The gravitational acceleration is 9.81 m/s²

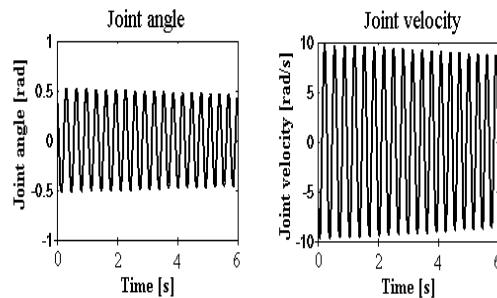


Figure 3.4: Behavior of limb if there is no force in muscles and there is 200 N vertically down load at the tip of the limb.

Verification of level of muscle In the next test case we use only one muscle: flexor or extensor. Flexor muscle tries to increase the joint angle and joint velocity while the extensor muscle tries to decrease the joint angle and joint velocity. In all cases the initial joint angle is 30 [degree], initial joint velocity is 0 [rad/s].

Movement of limb: little constant force in flexor fiber without tendon and pennation

One joint with one flexor and extensor muscle containing one kind of fiber and sarcomere. There is little 10 N constant force in flexor muscle and there is not force in extensor muscle. Gravitational acceleration is 9.81 m/s². Initial joint angle is 30°, initial joint velocity is 0 rad/s.

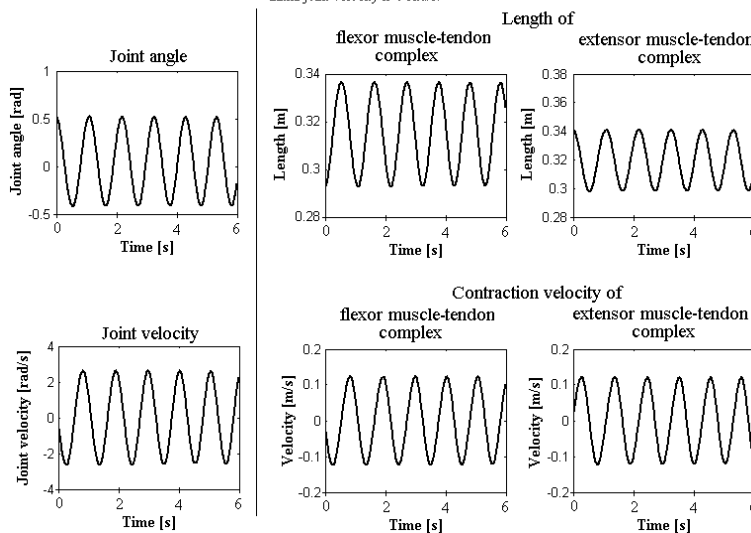


Figure 3.5: Little constant force in the flexor muscle. Limb moves like a pendulum but the equilibrium is at positive joint angle.

The case of flexor muscle. If the flexor muscle is excited by weak neuronal input then we expect that the movement of limb is the same as in the case of no forces (like a pendulum), but the equilibrium is not at zero joint angle, but it is at a little positive joint angle. The joint angle and joint velocity of this movement is displayed in fig.3.5. As we expected, the joint angle and joint velocity change sinusoidally and

the equilibrium is approximately at the angle 0.1 rad. During the simulation the gravitational acceleration is 9.81 [m/s²] and the force of muscle is 10 [N].

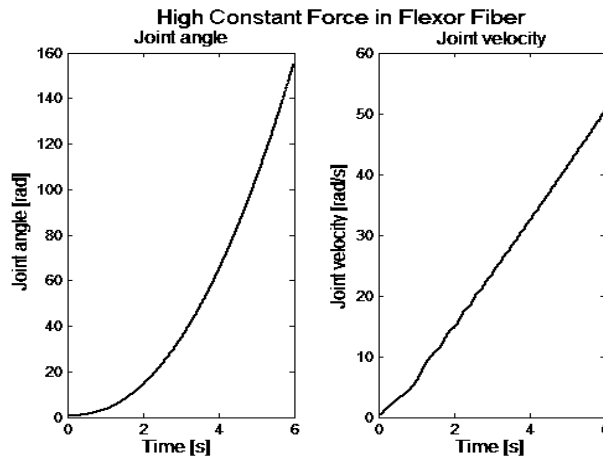


Figure 3.6: High constant force in the flexor muscle while there is no constraint range of motion. Joint rotates in the positive direction at higher and higher velocity.

If the flexor muscle is excited by high neuronal input then we expect that the movement of limb is not like a pendulum movement any more. Instead, the joint angles and joint velocity increase continuously if there is no constraint range of motion, or the joint angle and joint velocity increase while the joint angle does not reach its limit. If the joint angle reaches the constraint range of motion then the joint angle does not increase any more and remain at its limit value while the joint velocity drops to zero. The joint angle and joint velocity of this movement is displayed in fig.3.6 without constraint range of motion. As we expected, the joint angle and joint velocity increase continuously. During the simulation the gravitational acceleration is 1.1 [m/s²] and the force of muscle is 50 [N].

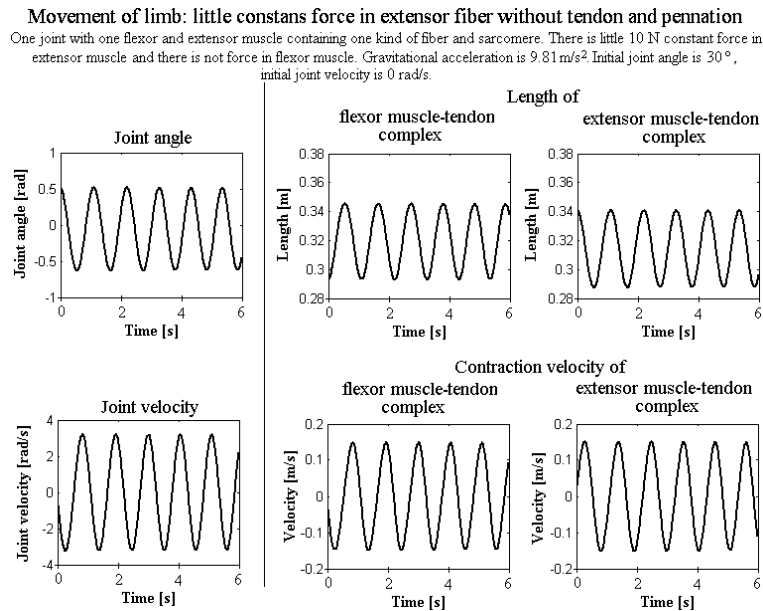


Figure 3.7: Little constant force in the extensor muscle. Limb moves like a pendulum but the equilibrium is at negative joint angle.

The case of extensor muscle. If the extensor muscle is excited by weak neuronal input then we expect that the movement of limb is the same as in the case of no forces (like a pendulum), but the equilibrium is not at zero joint angle, but it is at a little negative joint angle. The joint angle and joint velocity of this

movement is displayed in fig.3.7. As we expected, the joint angle and joint velocity change sinusoidally and the equilibrium is approximately at the angle -0.1 rad. During the simulation the gravitational acceleration is 9.81 $[m/s^2]$ and the force of muscle is 10 $[N]$.

If the extensor muscle is excited by high neuronal input then we expect that the movement of limb is not like a pendulum movement any more. Instead, the joint angles and joint velocity decrease continuously if there is no constraint range of motion, or the joint angle and joint velocity increase while the joint angle does not reach its limit. If the joint angle reaches the constraint range of motion then the joint angle does not decrease any more and remain at its limit value while the joint velocity drops to zero. The joint angle and joint velocity of this movement is displayed in fig.3.8 without constraint range of motion. As we expected, the joint angle and joint velocity decrease continuously. During the simulation the gravitational acceleration is 1.1 $[m/s^2]$ and the force of muscle is 50 $[N]$.

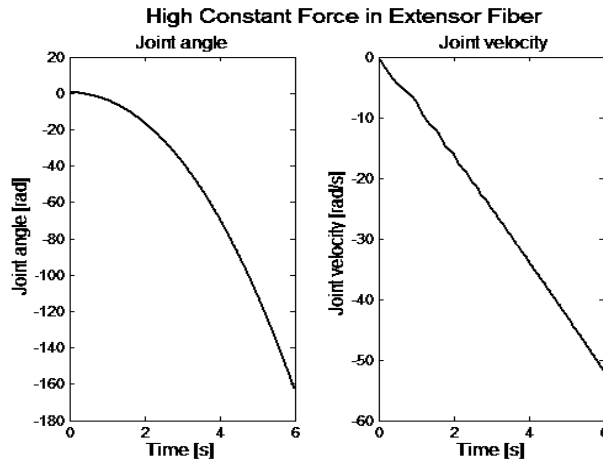


Figure 3.8: *High constant force in the extensor muscle while there is not constraint range of motion. Joint rotates in the negative direction at higher and higher velocity.*

In more complex cases, when the muscle contains more fibers, the main characteristics of these movements will not change.

Verification of the level of fiber and level of sarcomere In this case all levels are functioning except for the sub-level of tendon and sub-level of aponeurosis.

In the example show here we examine the activation frequency generation of fibers. This example shows that although the activation signal is very simple, the movement pattern is quite complex. The simulated result of this example is shown in fig.3.9. In this figure the time variation of most variables of the limb and muscles are shown such as: the length and the contraction velocity of muscle-tendon complexes, muscles, fibers and sarcomeres, the forces of muscle, fiber and sarcomere, the torque of muscle, the activation signal and the exciting frequency of fibers. We note that there are algebraic relationships between the length, contraction velocity and force of muscle, fiber and sarcomere. These variables are shown only for the sake of completeness.

In this example we use the same limb as before but the activation signal of the flexor muscle is a sinus function while the activation signal of the extensor muscle is the cosine function as it is seen in the right hand corner of the figure. There is no tendon and no pennation. The minimal exciting frequency of the fibers is 5 Hz while the maximal exciting frequency of the fibers is 15 Hz. The threshold activation level is 0.8 in case of both muscles. Both muscles contains only one fiber. In the figure it is seen that the exciting frequency of the fibers are not zero only if the activation level of the muscle is higher or equal than the threshold activation level of the current muscle.

Verification of the level of tendon In order to investigate the effect of tendon, we first generate a simple movement of the simplest limb. During this movement the activation signal of flexor muscle is constant 0.9 while the activation signal of extensor muscle is constant 0 . The threshold activation level is 0.8 in case of both muscles. The initial joint angle is 30 [degree] while the initial joint velocity is -2 [rad/s], i.e. the

Movement of limb: sinusoidal excitation without tendon and pennation

There are one joint with one flexor and one extensor muscle containing one kind of fiber and sarcomere. The gravitational acceleration is 9.81 m/s^2 . Initial condition: initial joint angle is 30° , and initial joint velocity is 0 rad/s .

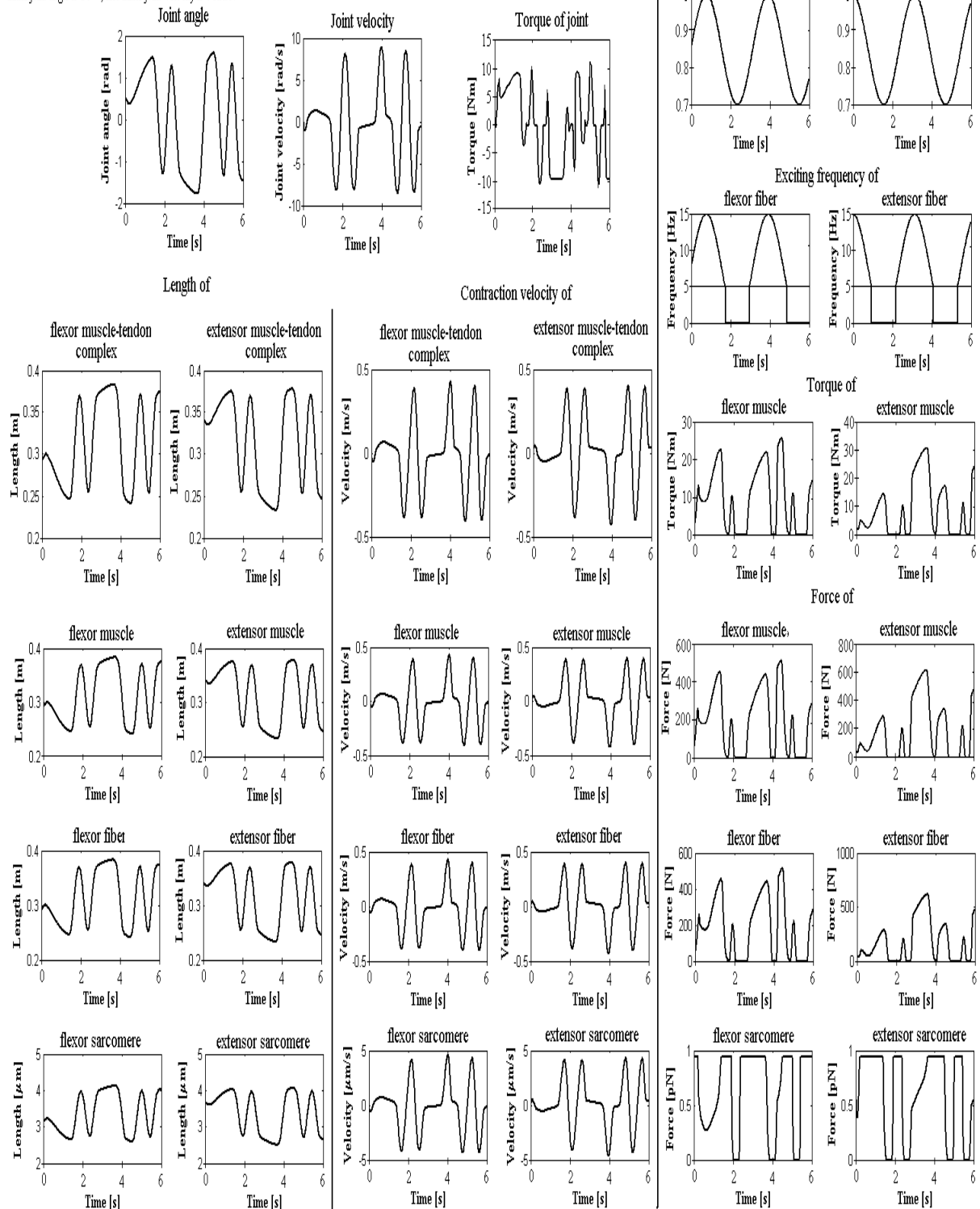


Figure 3.9: The activation signal of flexor is a sinus function while the activation signal of the extensor muscle is a cosine function.

joint angle decreases initially. We expect that the joint angle start to increase as an effect of force in flexor muscle as far as the torque of flexor muscle and the torque of gravitational force become equal. In fig.3.10 this behavior is shown.

Movement of limb: constant activation signal in flexor fiber without tendon and pennation

There is one joint with one flexor and one extensor muscle containing one kind of fiber and sarcomere. Flexor muscle has got const. 0.9 activation signal. Gravitational acceleration is 9.81 m/s^2 . Initial joint angle is 30° and initial joint velocity is -2 rad/s .

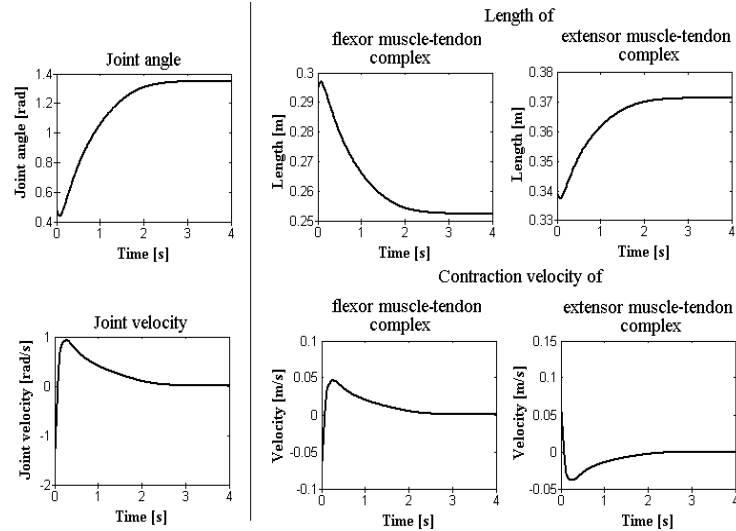


Figure 3.10: *The activation signal of the flexor muscle is constant 0.9 while the extensor muscle doesn't get any activation.*

What changes if muscles have got tendons but except for this, the limb remains the same as before? The tendons are in extended position initially since their resting lengths are 3 cm but their initial lengths are 5 cm. The same activation signal is given to the muscles as previously. In fig.3.11. One see that the torque of joint is increased but mainly the properties of extensor muscle are changed dramatically. It is also seen that the length of tendons change as far as they reach an equilibrium. As the effect of tendon one observes that the equilibrium of the joint angle and the contraction velocity changes, both increase.

Movement of limb: constant activation signal in flexor fiber with tendon and without pennation

There is one joint with one flexor and one extensor muscle containing one kind of fiber and sarcomere. Flexor muscle has got const. 0.9 activation signal. Gravitational acceleration is 9.81 m/s^2 . Initial joint angle is 30° and initial joint velocity is -2 rad/s . Both tendon are extended initially (5 cm while rest is 3 cm)

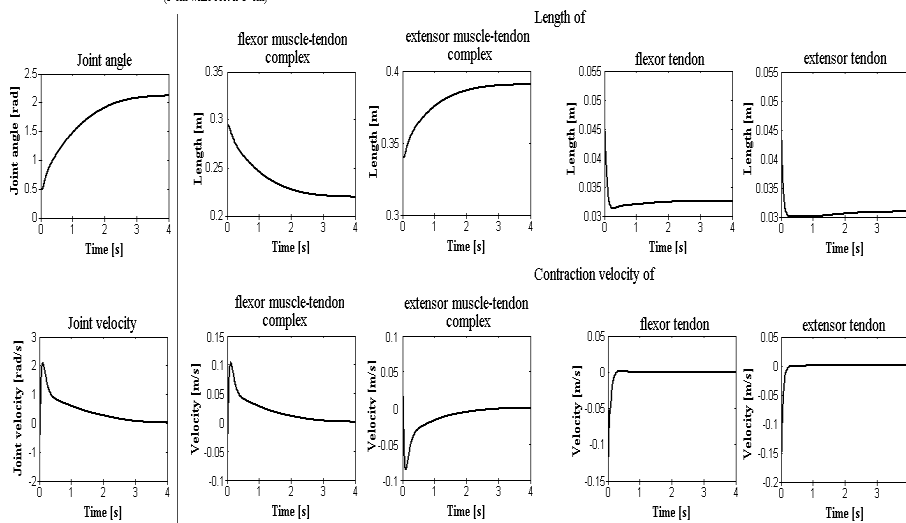


Figure 3.11: The activation signal and the limb are the same as in fig.3.10 except for both muscles have got tendons what are extended initially.

Chapter 4

Conclusion and future work

Our aim was to create an integrating framework of a model of limb that can handle any kind of sub-models of various processes. Therefore, a multilevel limb model has been constructed where each level represents a physiologically and/or anatomically important part of the real limb. They are the level of sarcomere, level of fiber or motor unit, level of muscle containing the sub-level of tendon and sub-level of aponeurosis, and the level of limb. This construction makes it possible to describe that the limb contains many serially connected segments and many muscles that rotate a joint. It means that our model can handle a lot of different kind of models of limbs and it is easily configurable according to the requirements of the expert.

To use of the proposed framework is demonstrated by using a simple yet realistic model of a real two-segment limb. The computational properties (such as degree of freedom and differential index) of the developed model has been investigated and model verification has been performed.

Basis on the model verification we have found that the dynamics of the model behaves as we expect. So we can continue the investigation of the details and estimate parameters of the model. Our next task is to examine the sensitivity of model with respect to its parameters. This step will hopefully lead to the decrease of the number of significant parameters since our model contains too many parameters for successful identification.

After the sensitivity analysis the parameter estimation test cases will be created and the planned test movements will be measured. By using the measured values the unknown parameter values will be estimated and finally the model will be validated.

Further work will be also directed towards extending our model to the 3D case.

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