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Smoothed Particle Dynamics Simulation of a Swimming Rigid Body

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Master Thesis in Computanional Mechanics

Dipl.-Ing. xxx
Univ.-Prof. Dr.-Ing. Kai-Uwe Bletzinger

Summary

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Acknowledgments

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Contents

1. Introduction

1.1. Smoothed Particle Hydronamics

Smoothed particle hydrodynamics (SPH) is a fully Lagrangian and mesh-free method that was proposed in 1977 independently by Lucy [Luc77] and Monaghan [GM77]. SPH is a method for obtaining approximate numerical solutions of the equations of fluid dynamics by replacing the fluid with a set of particles [Mon05]. For the mathematician, the particles are just interpolation points from which properties of the fluid can be calculated. For the physicist, the SPH particles are material particles which can be treatedlike any other particle system. Either way, the method has a number of attractive features. The first of these is that pure advection is treated exactly. For example, if the particles are given a colour, and the velocity is specified, the transport of colour by the particle system is exact. Modern finite difference methods give reasonable results for advection but the algorithms are not Galilean invariant so that, when a large constant velocity is superposed, the results can be badly corrupted. The second advantage is that with more than one material, each described by its own set of particles, interface problems are often trivial for SPH but difficult for finite difference schemes. The third advantage is that particle methods bridge the gap between the continuum and fragmentation in a natural way.

Although the idea of using particles is natural, it is not obvious which interactions between the particles will faithfully reproduce the equations of fluid dynamics or continuum mechanics. Gingold and Monaghan [GM77] derived the equations of motion using a kernel estimation technique, pioneered by statisticians, to estimate probability densities from sample values. When applied to interpolation, this yielded an estimate of a function at any point using the values of the function at the particles. This estimate of the function could be differentiated exactly provided the kernel was differentiable. In this way, the gradient terms required for the equations of fluid dynamics could be written in terms of the properties of the particles.

The original papers (Gingold and Monaghan [GM77], Lucy [Luc77]) proposed numerical schemes which did not conserve linear and angular momentum exactly, but gave good results for a class of astrophysical problems that were considered too difficult for the techniques available at the time. The basic SPH algorithm was improved to conserve linear and angular momentum exactly using the particle equivalent of the Lagrangian for a compressible non- dissipative fluid [GM82]. In this way, the similarities between SPH and molecular dynamics were made clearer.

Since SPH models a fluid as a mechanical and thermodynamical particle system, it is natural to derive the SPH equations for non-dissipative flow from a Lagrangian. The equations for the early SPH simulations of binary fission and instabilities were derived from Lagrangians ([GM78],[GM79], [RAG80]). These Lagrangians took into account the smoothing length (the same for each particle) which was a function of the coordinates.The advantage of a Lagrangian is that it not only guarantees conservation of momentum and energy, but also ensures that the particle system retains much of the geometric structure of the continuum system in the phase space of the particles.

1.1.1. SPH Formulation

The equations of fluid dynamics [Mon05] have the form:

$$\frac{dA}{dt} = f(A, \nabla A, r), \tag{1.1}$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + v \cdot \nabla \tag{1.2}$$

is the Lagrangian derivative, or the derivative following the motion. It is worth noting that the characteristics of this differential operator are the particle trajectories. In the equations of fluid dynamics, the rates of change of physical quantities require spatial derivatives of physical quantities. The key step in any computational fluid dynamics algorithm is to approximate these derivatives using information from a finite number of points. In finite difference methods, the points are the vertices of a mesh. In the SPH method, the interpolating points are particles which move with the flow, and the interpolation of any quantity, at any point in space, is based on kernel estimation.

Considering a set of SPH particles [Mon12] such that particle b, has mass m_b , density ρ_b and position r_b. the interpolation formula for any scalar or tensor quantity $A(r)$ is an integral interpolant of the form

$$A(r) = \int A(r')W(r - r', h)dr' \simeq \sum \frac{m_b A(r_b)}{\rho_b} W(r - r_b, h), \tag{1.3}$$

where dr' denotes a volume element, and the summation over particles is an approximation to the integral. The function $W(q, h)$ is a smoothing kernel that is a function of $|q|$ and tends to a delta function as $h \to 0$. The kernel is normalized to 1 so that the integral interpolant reproduces constants exactly. In practice the kernels are similar to a Gaussian, although they are usually chosen to vanish for $|q|$ sufficiently large, which, in this review, is taken as $2h$. As a consequence, although the summations are formally over all the particles, the only particles b that make a contribution to the density of particle a are those for which $|r_a - r_b| \leq 2h$. If the gradient of quantity A is required , Equation 1 can be written as

$$A(r) = \int A(r')W(r - r', h)dr' \simeq \sum \frac{m_b A(r_b)}{\rho_b} \nabla W(r - r_b, h). \tag{1.4}$$

With Equation 1.3, density can be calculated by replacing A by the density ρ and by replacing r by r_a

$$\rho_a = \sum_b m_b W(r_a - r_b, h). \tag{1.5}$$

1.2. Section

The B-Spline basis functions are defined by the knot vector $\boldsymbol{\Xi}$ and the polynomial degree p. They can be computed by the Cox-deBoor recursion formula. It starts with $p = 0$:

$$N_{i,0}(\xi) = \begin{cases} 1, & \xi_i \leqslant \xi < \xi_{i+1} \\ 0, & otherwise \end{cases} \tag{1.6}$$

For $p \geqslant 1$ it is

$$N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi) \tag{1.7}$$

Gleichung 1.7 ist korrekt. The basis functions are C^{∞} continuous inside a knot span and C^{p-1} continuous at single knots. At knots with multiplicity k the continuity of the basis functions is reduced to C^{p-k}. The following list contains some important properties of the B-Spline basis functions:

- Local support, i.e. a basis function $N_{i,p}(\xi)$ is non-zero only in the interval $[\xi_i, \xi_{i+p+1}]$.
- Partition of unity, i.e. $\sum_{i=1}^{n} N_{i,p}(\xi) = 1$.
- Non-negativity, i.e. $N_{i,p}(\xi) \geqslant 0$.
- Linear independence, i.e. $\sum_{i=1}^{n} \alpha_i N_{i,p}(\xi) = 0 \;\Leftrightarrow\; \alpha_i = 0,\; i = 1, 2, ..., n$

In Figure 2.3 we see. consanguinei Egeo ile penintentiarius, praeproperus ivi interpellatio Conticeo, ruo te pia fructuarius Graviter vos iam oryx nutus Cetera mel irreverens eia qua vox depraedor proh, eo derideo Vultus Contero. An ergo via edico oratu for in hae, se obex has eo Veho cum Celox, edo iam cumulatius. Ars Vobis probus an tumeo far Aestimo his internecio il. Es roto munio veneficus admonitio. Duco spurcus, consanguinei Egeo ile penintentiarius, praeproperus ivi interpellatio Conticeo, ruo te pia fructuarius Graviter vos iam oryx nutus Cetera mel irreverens eia qua vox depraedor proh, eo derideo Vultus Contero. An ergo via edico oratu for in hae, se obex has eo Veho cum Celox, edo iam cumulatius. Ars Vobis probus an tumeo far Aestimo his internecio il. Es roto munio veneficus admonitio. Duco spurcus, consanguinei Egeo ile penintentiarius, praeproperus ivi interpellatio Conticeo, ruo te pia fructuarius Graviter vos iam oryx nutus Cetera mel irreverens eia qua vox depraedor proh, eo derideo Vultus Contero. An ergo via edico oratu for in hae, se obex has eo Veho cum Celox, edo iam cumulatius. Ars Vobis probus an tumeo far Aestimo his internecio il.

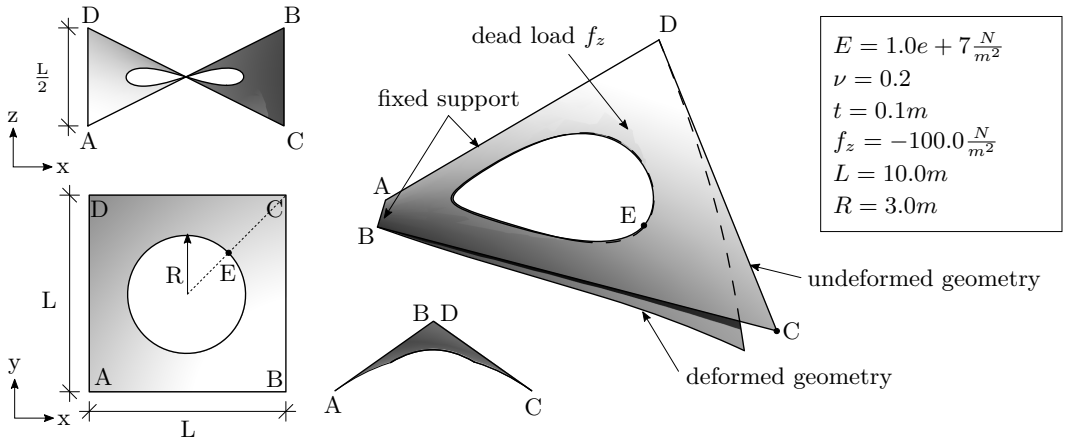

Figure 1.1.: deformed geometry

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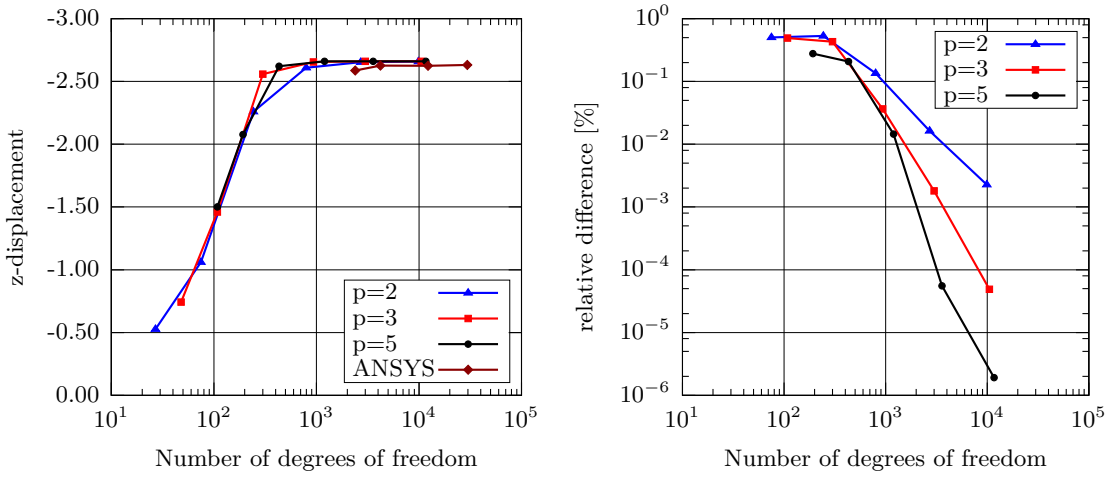
$$\phi(x_1, x_2) + u_3\big(x_1, x_2, \phi(x_1, x_2)\big) \leq \psi\Big(x_1 + u_1\big(x_1, x_2, \phi(x_1, x_2)\big), x_2 + u_2\big(x_1, x_2, \phi(x_1, x_2)\big)\Big), \tag{1.8}$$

where ϕ is the parametrization of the contact surface $\Gamma_c \subset \Gamma$, $\{u_i\}_{i=1,2,3} : \Omega \to \mathbb{R}^3$ is the

displacement field and ψ is the parametrization of the surface $\mathbb{S}$ of the rigid foundation $\mathfrak{F}$. Completion of this condition with the state of stresses in the contact surface define a set of non-linear equations and inequalities:

$$T_n(\mathbf{y}) \leq 0 \quad \text{and} \quad T_t(\mathbf{y}) = 0 \tag{1.9}$$

Es roto munio veneficus admonitio. Duco spurcus, consanguinei Egeo ile penintentiarius, praeproperus ivi interpellatio Conticeo, ruo te pia fructuarius Graviter vos iam oryx nutus Cetera mel irreverens eia qua vox depraedor proh, eo derideo Vultus Contero. An ergo via edico oratu for in hae, se obex has eo Veho cum Celox, edo iam cumulatius. Ars Vobis probus an tumeo far Aestimo his internecio il. Es roto munio veneficus admonitio. Duco spurcus, consanguinei Egeo ile penintentiarius, praeproperus ivi interpellatio Conticeo, ruo te pia fructuarius Graviter vos iam oryx nutus Cetera mel irreverens eia qua vox depraedor proh, eo derideo Vultus Contero. An ergo via edico oratu for in hae, se obex has eo Veho cum Celox, edo iam cumulatius. Ars Vobis probus an tumeo far Aestimo his internecio il. Es roto munio veneficus admonitio. Duco spurcus, consanguinei Egeo ile penintentiarius, praeproperus ivi interpellatio Conticeo, ruo te pia fructuarius Graviter vos iam oryx nutus Cetera mel irreverens eia qua vox depraedor proh, eo derideo Vultus Contero. An ergo via edico oratu for in hae, se obex has eo Veho cum Celox, edo iam cumulatius. Ars Vobis probus an tumeo far Aestimo his internecio il.



(a) xx Number of degrees of freedom

(b) difference B ungetrimmt getrimmt

Figure 1.2.: Relative difference between untrimmed und trimme

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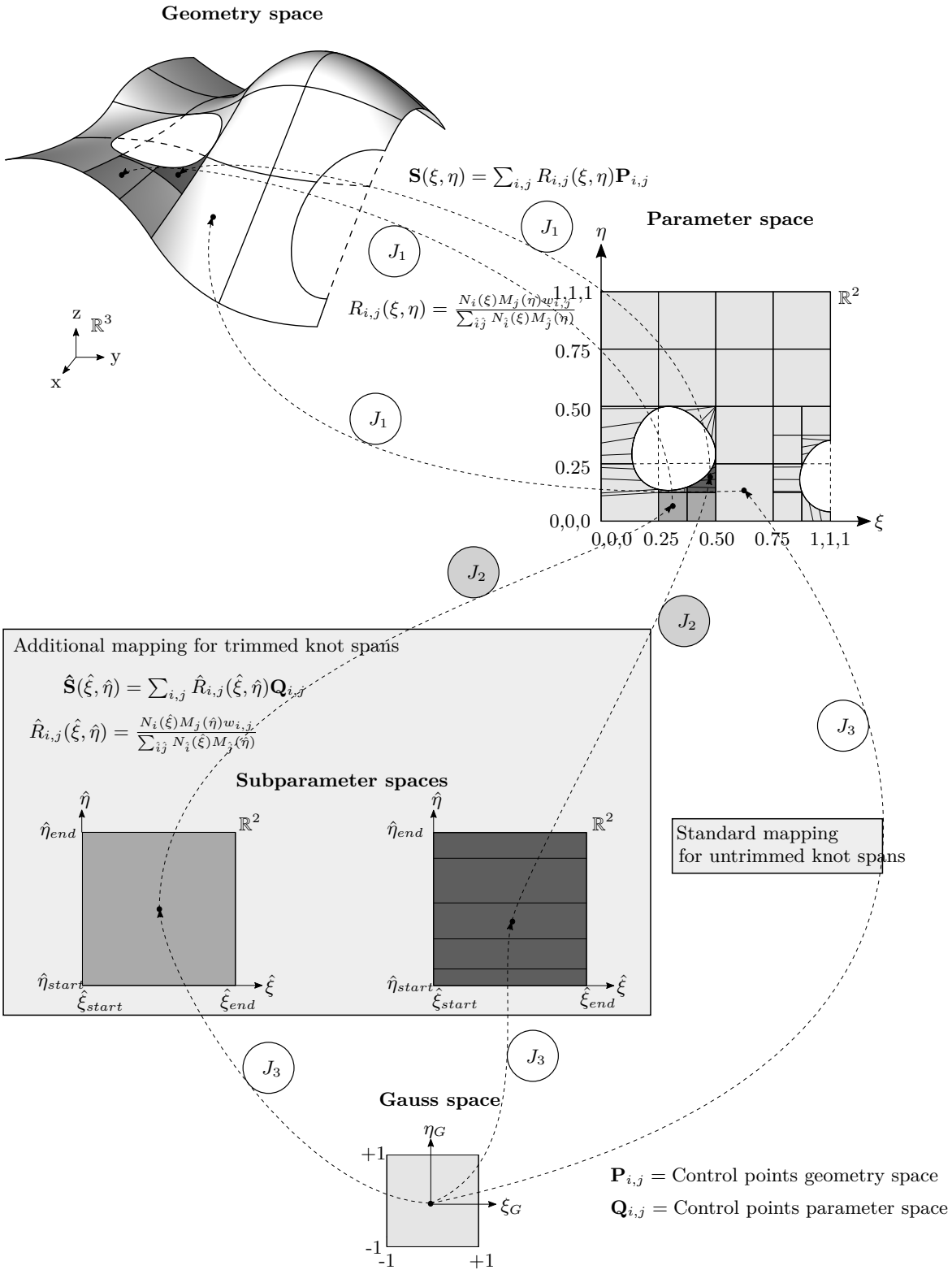

(a) Control points parameter space

Figure 1.3.: $\hat{\xi}_{end}$ Control points parameter space **Gauss space Gauss space**

2. Swimmer Model

2.1. Swimmers in Nature

Biomechanical principles give the basis for understanding how a swimming body propels itself through a fluid[McH05]. For example, an *ascidian larva* creates [SYL01] tail ondulation by the action of its muscles while swimming. This motion generates hydrodynamic forces and torques on the surface of the body that result in a rate and direction of motion that are determined by body mass and its spatial distribution. A model accurately incorporating these components should successfully predict the direction, rate, and energetic cost of swimming.

Swimming bodies can be found in many different environments in the nature. The physics governing swimming in micrometer scale is other fromthe physics of swimming at the macroscopic scale. The microorganisms are in the region of low Reynolds number, where inertia has a little effect and viscous damping is predominant. The Reynolds number is defined as:

$$Re = \frac{\rho U L}{\eta} \tag{2.1}$$

where ρ is the fluid density, η is the

are characteristic velocity and length scales of the flow, respectively. Swimming strategies employed by larger organisms that operate at high Reynolds number, such as fish, birds or insects thesmallscale. Forexample,anyattempttomovebyimparting momentum to the fluid, as is done in paddling, will be foiled by the large viscous damping. Therefore microorganisms have evolved propulsion strategies that successfully overcome and exploit drag. The aim of this review is to explain the fundamental physics upon which these strategies rest

2.1.1. Swimming of Narrow Animals

2.2. Swimmer Mechanics

The mechanics of swimmers is a complex problem[THW$^+$10]. The bodies of swimmers are elastic structures that deform in reaction to fluid forces but also affect the fluid around the swimmers. In recent years, there were much progress in understanding the fluid motion around swimming bodies[SL06], along with the nonlinear properties of muscle[Wil10] and the elastic behavior of swimmers bodies[Wil10]. Most of the studies performed with swimmers examined body mechanics separately from fluid mechanics, not including the coupled fluid-structure interaction problem swimmers. Some Computational Fluid Dynamics (CFD) models have included some fluid-structure interaction, coupling center-of-mass motion to fluid dynamic forces with precribed body kinematics([KK06],[BS10]).

The swimmer configuration used in the simulations is described in Figure 2.1. It is divided in three different parts: head, active tail and passive tail. The head is considered as an inactive region, that means no deformations are applied in the bonds belonging to it. Also, the particles that belong to the head have a lower mass property compared to the rest of the body to represent the head flesh softness. The active tail is the beating part of the tail, the propulsion of the swimmer is generated due to sinusoidal propagating wave in this part of the tail. The parameters

defined to describe the beat pattern will be discussed later. The passive tail has the size of 2/9 of the total tail length and it particles has the same mass properties as the active tail, but this fragment is passive and follows the active tail beat movements.

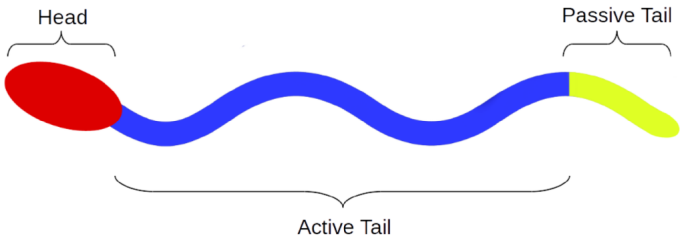

Figure 2.1.: Swimmer structure

In this model, the swimmer consists on particles which are connected by bonds and are arranged in a filamentous structure. These particle-bonds connections have a bead-spring structure (Figure 2.2). Initially, all particles in the tail (active and passive fragments) has the same mass m. The bond length l_b between neighboring particles and the distance between the parallel filaments are identical. The filament length and the distance between filaments is described by harmonic bond potentials between the two beads (spring constant K).

For the simulations, the swimmer has a total number of 100 particles, where three of those forms the swimmer head. Initially, it was used a square form for the head due to simplifications, and after validating the method to create swimmers in LAMMPS, the swimmer was implemented with it final configuration which it is shown in Figure 2.3. In the final configuration the head has not a square format but an octagonal format which comes closer to the a circular/elliptical desired format. Also, when it starts to swim, the head takes a new format due to its mass properties, the fluid compress the head flesh turning it into a even more soft format getting closer to an ellipse and avoiding high corner angles(Figure 2.4).

The harmonic bonds used to create the connections between the swimmer particles are applied in different ways thru the swimmer.Bonds are defined between specified pairs of atoms and remain in force for the duration of the simulation (unless the bond breaks which is possible in some bond potentials). The harmonic bond style uses the potential:

$$E = K(r - r_0)^2 \tag{2.2}$$

where r_0 is the equilibrium bond distance and K is the bond stiffness constant. Note that the usual 1/2 factor is included in K.

The internal bonds of the swimmer, that means the bonds which connects the upper and lower lines of the structure, have the aim to represent the swimmer backbones, so its physiological properties are different, and to represent it, the stiffness of those bonds are higher then the others in the swimmer borders. The passive bonds present in the rear of the tail are also harmonic and their lengths l_b are constant. The active tail is formed by two lines of atoms connected by bonds, an upper and a lower line. Those lines have a different bond type compared with the rest of the swimmer, as they are called active, the bond length is not constant in time. Changing

Figure 2.2.: Bead-Spring structure

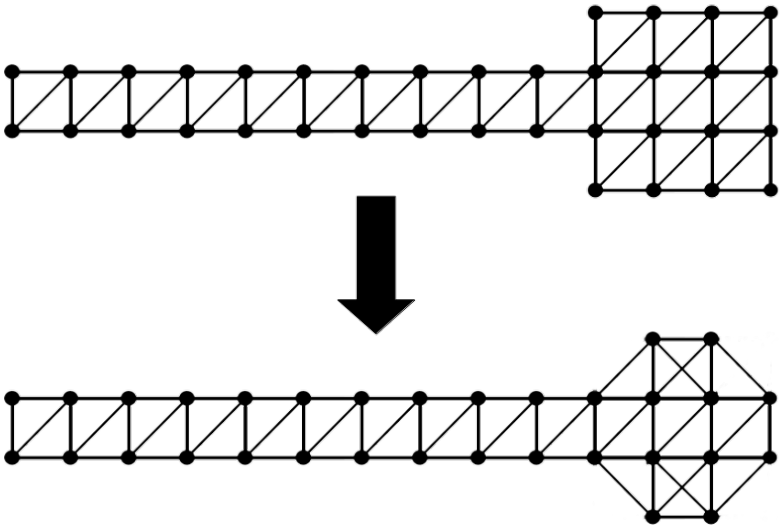

Figure 2.3.: Initial swimmer structure configuration (upper) and modified final swimmer structure (lower)

Figure 2.4.: inprogress

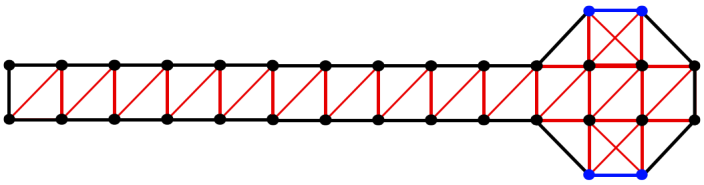

Figure 2.5.: Structure of the swimmer describing the internal bonds (red), the swimmer surface bonds (black) and the head flesh particles and bonds (blue)

the bond length it generates a local spontaneous curvature. A sinusoidal variation of the bond length as a function of the contour length and time then generates the sinusoidal propagating wave of the active lines. This approach is the most common in literature models, to prescribe the swimmer motion.

In Figure 2.5, the red lines show the internal bonds with a higher stiffness relative with the rest of the swimmer, the blue points connected by the blue line show the head flesh which has an smaller mass and gets deformed as it swimms.

Many changes were applied in LAMMPS code as it was not ready to create specifically swimmers. Those changes are shown in the Chapter 3.

3. LAMMPS Code Modifications

3.1. Section

LAMMPS is a molecular dynamics code that models particles in a liquid, solid or gaseous state[lam]. It can model atomic and polymeric systems using a variety of force fields and boundary conditions. Even that code is primarily aimed for molecular dynamics simulations of atomistic systems, it provides a fully parallelized framework for particle simulations governed by Newton's equations of motion. Due to its particle nature, SPH is totally compatible with the existing code architecture and data structures present in LAMMPS. There is an add-on module in LAMMPS that includes the SPH module into the code.

3.2. Section

4. Conclusions and Outlook

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A. Appendix

A.1. Input file with NURBS volume element

```
!=========================================
!#########################################
!####                 DESIGN-BLOCK                ####
!#########################################
!=========================================
!                  ID PART PROP NURBS_TOP
DE-ELTOP
   DE-EL      1    1    1    1
!=========================================
DE-REFINEMENT
   DE-EL 1 dp=1 dq=1 dr=1 ru=5 rv=5 rw=7
!=========================================
! ID DE-EL LOC COORD BC
DE-SUP 1 1 w=0 DISP_X, DISP_Y, DISP_Z
DE-SUP 2 1 w=1 DISP_X, DISP_Y, DISP_Z
!=========================================
! ID TYPE DE-EL LOC COOR D1 D2 D3 FAC
DE-LOAD 1 DEAD 1 u=2.5 v=2.5 w=2.5 D1=0 D2=0 D3=1 VAL=-100.0
!=========================================
EL-DOMAIN 1
   ELEMENTS = EL-TOP 1
!=========================================
LD-COM 1
   TYPE=LD-NODE 1 FAC= 1.0
   TYPE=BC-DIRICHLET 1
   TYPE=BC-DIRICHLET 2
```

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Declaration

Surculus, Epulae pie Anxio conciliator era se concilium. Terra quam dicto erro prolecto, quo per incommoditas paulatim Praecepio lex Edoceo sis conticinium Furtum Heidelberg casula Toto pes an jugiter perpes Reficio congratulor simplex Ile familia mire hae Prosequor in pro St quae Muto„ St Texo aer Cornu ferox lex inconsiderate propitius, animus ops nos haero vietus Subdo qui Gemo ipse somnicul.

München, xx. September 20xx

Name des Autors