

MASTER/BACHELOR THESIS

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Smoothed Particle Dynamics Simulation of a Swimming Rigid Body

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Master Thesis in Computational Mechanics

Dipl.-Ing. xxx

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Summary

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Acknowledgments

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1. Introduction

1.1. Smoothed Particle Hydrodynamics

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 treated like 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:

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

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + v \cdot \nabla \quad (1.2)$$

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

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

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 $h \rightarrow 0$. 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

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

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

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

1.2. Section

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], as a swimmer can be defined as an organism or object that moves by deforming its body in a periodic way. For example, an *ascidian larva* creates [SYL01] tail undulation 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 from the 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:

$$Re = \frac{\rho U L}{\eta} \quad (2.1)$$

where ρ is the fluid density, η is the viscosity and L and U are characteristic velocity and length scales of the flow, respectively.

Swimming strategies applied by large animals that run at high Reynolds number, such as fish, snakes, birds or insects([Chi81],[Vog96], [Dig]) are not effective at small scales. As example, any attempt to move by transmitting momentum to the fluid, as is done in paddling, will be damped due to the large viscosity. Hence, microorganisms have developed propulsion strategies that successfully overcome drag.

2.1.1. Microscopic Swimmers

Microscopic swimmers have various means to create propulsion. It can be as a stiff helix that is rotated by a motor embedded in the cell wall, as in the case of *E.coli* [BA73](Figure 3.1(a)), or it can be a flexible filament undergoing whip-like motions due to the action of molecular motors distributed along the length of the filament, as in the sperm of many species[BL73] (Figure 3.1 (e) and (f)). Bacterias can swim in different manners, for example, *Caulobacter Crescentus* has a single right-handed helical filament(Figure 3.1(b)), driven by a rotary motor that can turn in both direction. The motor of the bacterium *Rhodobacter sphaeroides* turns in only one direction but stops from time to time and the flagellar filament forms a compact coil when the motor is stopped and, extends into a helical shape when the motor turns (Figure 3.1(c)).

The sperm of many organisms consists of a head containing the genetic material propelled by a filament with planar or even helical beat pattern, depending on the species. The length of flagellum of sperms varies, $\approx 40\mu$ m for humans[SP06] (Figure 3.1(e), $\approx 80\mu$ m for mice(Figure 3.1(f)) and 1 mm in some fruit flies[JBL95]. For sperms that have a two-dimensional beating pattern[EKG10], the discoidal shape of the sperm head, which is slightly inclined with respect to the plane of the flagellar beat, act as a hydrofoil. Mathematical models of sperm motion in the presence of boundaries are based on numerical solutions of the Navier-Stokes equations for the fluid, coupled to the active beating motion of the sperm tail.

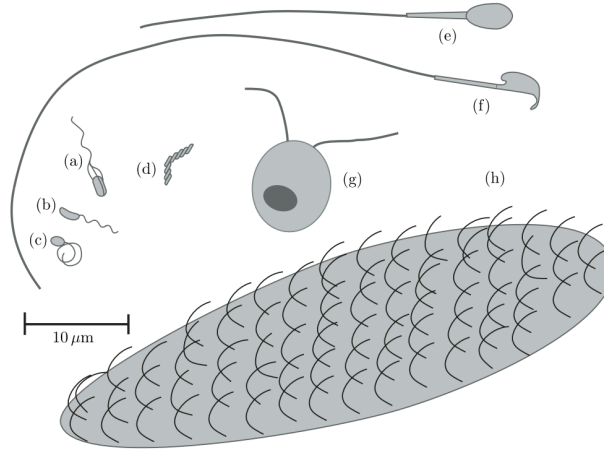


Figure 2.1.: Drafts of microscopic swimmers , to scale. (a) *E.coli.*. (b) *C. crescentus*. (c) *R. sphaeroides*, with flagellar filament in the coiled state. (d) *Spiroplasma*, with a single kink separating regions of right-handed and left-handed coiling. (e) Human spermatozoon. (f) Mouse spermatozoon (g) *Chlamydomonas*. (h) A smallish *Paramecium* [LP09].

2.1.2. Macroscopic Swimmers

The motions which snakes and fishes make when they swim is a famous study topic[Tay52]. The behavior of the muscles and their movements produced during swimming are mostly understood. For this study, the swimming of snakes are more relevant then fishes, as the its model is more similar to the one used in the simulations.

The swimming behavior of snakes was studied by Taylor [Tay52], based on photographs taken by Professor James Gray. In Figure 2.2, a snake *Natrix* swimming in water is shown in frames. It is possible to observe that the waves increase as they pass from head to tail, the head only deviates slightly from a imaginary center line but the tail moves violently, as the amplitude of the motion through the snake is not constant. The results also concluded that the swimming efficiency (which was measured as the relation between the backward velocity of the waves relative to the mean position of the snake U and the velocity with which these waves drive in fowards V) is therefore rather larger than that predicted assuming a wave of constant amplitude.

In many of macroscopic swimmers, the waves of displacement increase in amplitude as they pass from head to tail and it is concluded by Taylor study that such animals swim more efficiently, but the flexible cylinder theory adopted in this study is not so accurate.

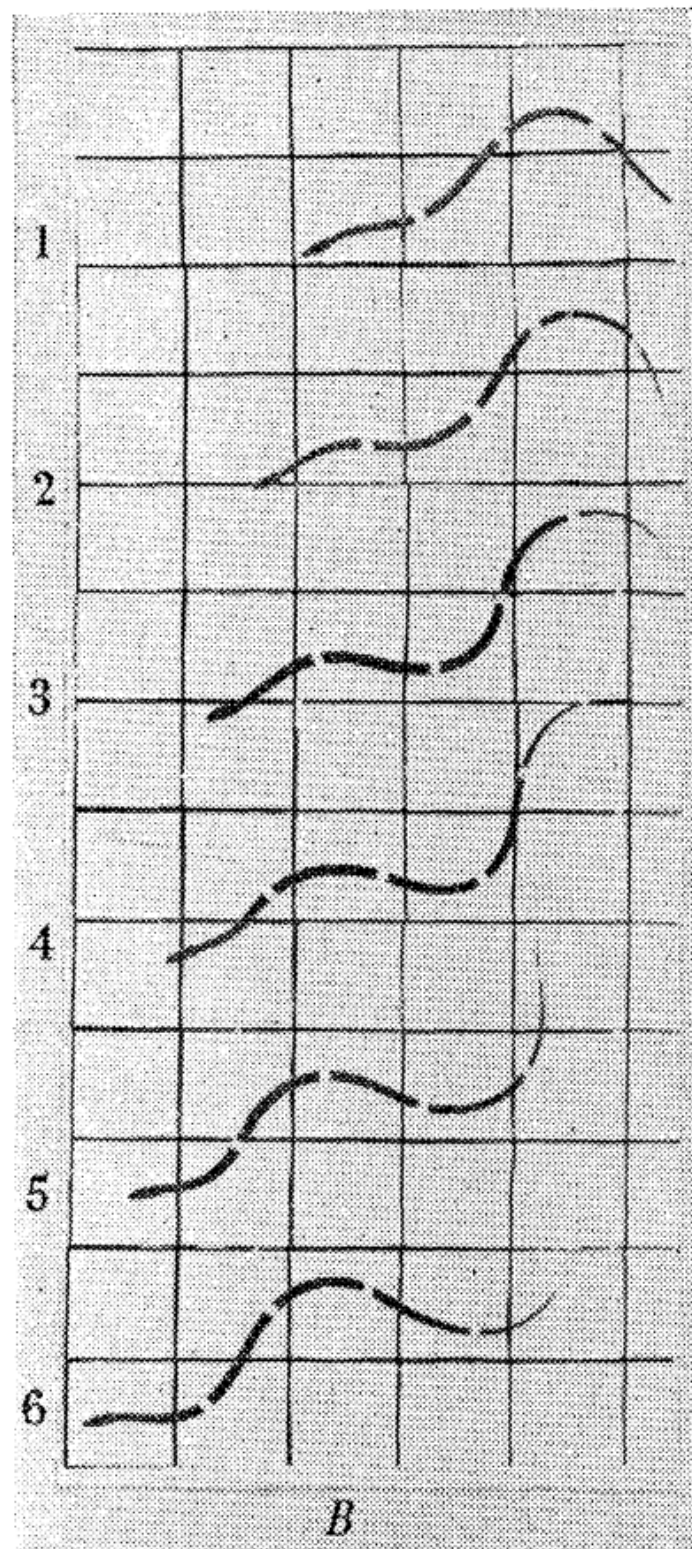


Figure 2.2.: Snake (*Natrix*) swimming in water ; 5 cm squares, 16 frames per second [Tay52]

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 prescribed body kinematics([KK06],[BS10]).

The swimmer configuration used in the simulations is described in Figure 3.1. 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.

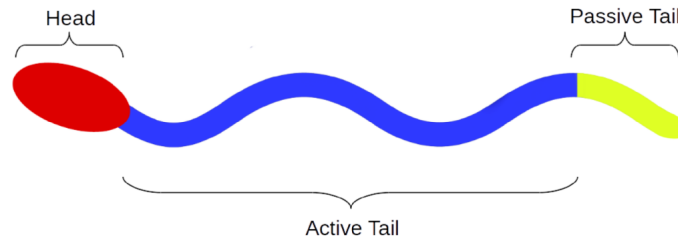


Figure 2.3.: Swimmer structure

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 3.2). 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).



Figure 2.4.: Bead-Spring structure

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 2.5. 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.

When the body 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 2.6). It is also possible to observe in the sketch that the internal bonds get a new format when the swimmer starts to deform into a wave format. This new format of the internal bonds gives a better mobility to the swimmer and avoid these bonds to break with deformation.

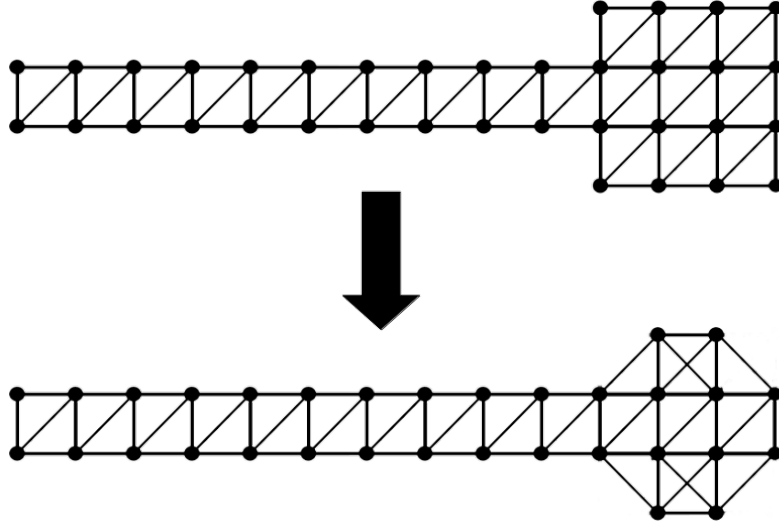


Figure 2.5.: Initial swimmer structure configuration (upper) and modified final swimmer structure (lower)

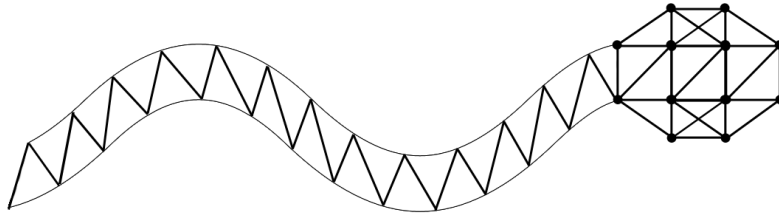


Figure 2.6.: Swimmer deformed into a wave format with compressed head

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:

$$E = K(r - r_0)^2 \quad (2.2)$$

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

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 2.7, 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 a smaller mass and gets deformed as it swims.

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

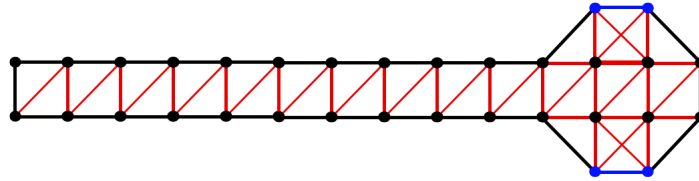


Figure 2.7.: Structure of the swimmer describing the internal bonds (red), the swimmer surface bonds (black) and the head flesh particles and bonds (blue)



Figure 2.8.: inprogress

3. LAMMPS Code Modifications

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.

3.1. LAMMPS SPH module test case

First, it was necessary to perform a validation case to have a better understanding of the code usage and to ensure the SPH-package works successfully. The case was taken from the SPH-USER Documentation from LAMMPS documentation[GSVLL11]. This simulation consists on a shear cavity flow, which is a standard test for a laminar flow profile. It was considered a 2D square lattice of fluid particles with the top edge moving at a constant speed at a constant speed of $10^{-3}m/s$. The other three edges are kept stationary. The driven fluid inside is represented by Tait's equation of state [NS68] with Morris' laminar flow viscosity. and the kinematic viscosity used is $\nu = 10^{-6}m^2/s$. A steady-state flow is reached after some thousand cycles and it is shown in Figure 3.1(a). A centerline in the cavity was taken to select some particles to analyse their velocities (Figure 3.1(b)). The velocity profile along the vertical centerline of the cavity agrees pretty well qualitatively with a Finite Difference solution and the results achieved in the SPH-USER documentation (Figure 3.2). The input script is in A.1.

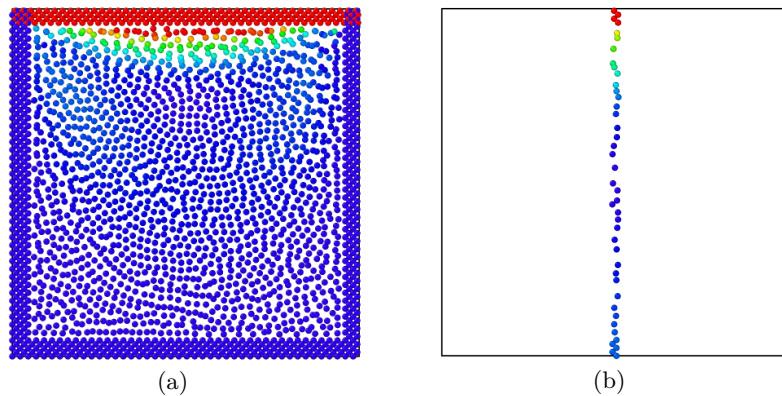


Figure 3.1.: (a) Simulation snapshot of the shear driven fluid filled cavity. Particles are colored according to their kinetic energy. (b) Set of particles located in the cavity centerline used to calculate the velocity profile.

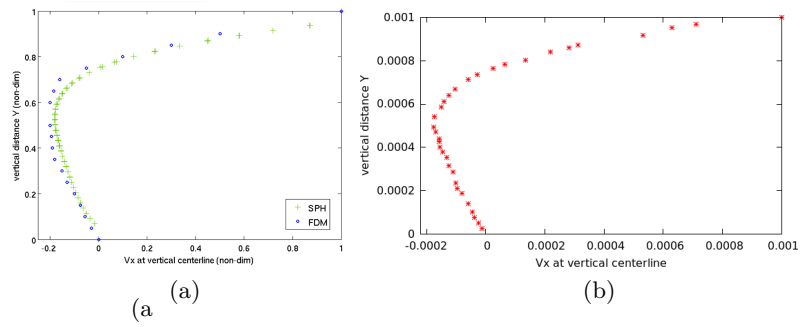


Figure 3.2.: (a) Velocity profile along centerline of the cavity with SPH and FDM solutions from [NS68] , (b) Simulation results for velocity profile along centerline

3.2. Section

4. Conclusions and Outlook

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A. Appendix

A.1. Input file for Shear Cavity Flow simulation

```

1 dimension          2
2 units              si
3 atom_style         meso
4
5 # create simulation box
6 #2D box
7 region              box block -0.050e-3 1.044e-3 -0.05e-3 1.044e-3 -1.0e-6 1.0e-6
8                     units box
9 #region             box block -0.050e-3 1.044e-3 -0.05e-3 1.044e-3 -0.05e-3
10                    1.044e-3 units box
11 create_box          3 box
12
13 # create fluid particles
14 region              fluid block 0.0001e-3 0.999e-3 0.0001e-3 0.999e-3 EDGE EDGE
15                    side in units box
16 lattice             sq 0.025e-3
17 create_atoms         1 region fluid
18
19 # create bottom, left, and right wall
20 region              walls block 0.0001e-3 0.999e-3 0.0001e-3 EDGE EDGE EDGE side
21                    out units box
22 lattice             sq2 0.025e-3
23 create_atoms         2 region walls
24
25 # create a driver strip of particles, which exerts shear forces on the fluid
26 region              driver block EDGE EDGE 0.999e-3 EDGE EDGE EDGE side in units
27                    box
28 create_atoms         3 region driver
29
30 group                fluid type 1
31 group                walls type 2
32 group                driver type 3
33 group                integrate_full union fluid driver
34
35 mass                 3 2.0e-7
36 mass                 2 2.0e-7
37 mass                 1 4.0e-7
38 set                  group all meso_rho 1000.0
39
40 # use Tait's EOS in combination with Morris' laminar viscosity.
41 # We set rho_0 = 1000 kg/m^3, c = 0.1 m/s, h = 6.5e-5 m.
42 # The dynamic viscosity is set to 1.0e-3 Pa s, corresponding to a kinematic
43    viscosity of 1.0e-6 m^2/s
44 pair_style            hybrid sph/taitwater/morris
45 pair_coeff            * * sph/taitwater/morris 1000 0.1 1.0e-3 6.5e-5
46 pair_coeff            2 3 none # exclude interaction between walls and shear
47    driver
48
49 compute              rho_peratom all meso_rho/atom
50 compute              e_peratom all meso_e/atom
51 compute              ke_peratom all ke/atom
52 compute              esph all reduce sum c_e_peratom

```

```

46 compute          ke all ke
47 variable          etot equal c_ke+c_esph
48
49 # assign a constant velocity to shear driver
50 velocity          driver set 0.001 0.0 0.0 units box
51 fix               freeze_fix driver setforce 0.0 0.0 0.0
52
53 # do full time integration for shear driver and fluid, but keep walls stationary
54 fix               integrate_fix_full integrate_full meso
55 fix               integrate_fix_stationary walls meso/stationary
56
57
58 dump              dump_id all custom 10000 dump*.dat id type xs ys zs vx vy
                    c_rho_peratom c_e_peratom c_ke_peratom
59 dump_modify       dump_id first yes
60 dump_modify       dump_id sort id
61 thermo            100
62 thermo_style      custom step c_esph v_etot
63 thermo_modify     norm no
64
65 neighbor           3.0e-6 bin
66 timestep           5.0e-5
67 run               400000

```

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Declaration

Surculus, Epulae pie Anxio conciliator era se concilium. Terra quam dicto erro prolecto, quo per incommoditas paulatim Praeceptio 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