

**This dataset contains all the simulation scripts, simulation results and postprocessing script for the manuscript “Hydrodynamic clustering of two finite-length flagellated swimmers in viscoelastic fluids”**

#### **About the folders:**

- The folder **“single\_withouthead”** contains all the simulation scripts and data for the study of the swimming velocity of a single swimmer. Here the swimmer has no head.
  - Inside this folder the **“mass”** folder contains the convergence study against Reynolds number.
  - The folder **“prescribing”** contains the study of a swimmer with prescribing waveform.
  - The folder **“vis”** contains the study of the swimming speed at different beating frequency and Deborah number.
- The folder **“single\_withhead”** contains all the simulation scripts and data for the study of the swimming velocity of a single swimmer. Here the swimmer has a head attached.
- The folder **“reciprocal”** contains the simulation scripts and data for the study of a swimmer beating in a reciprocal way.
- The folder **“convergence”** contains all the simulation scripts and data for the convergence test.
- The folder **“instability”** contains all the simulation scripts and data for the clustering instability study.
  - The folder **“instability/nohead/db”** contains instability study of two stiff swimmers.
  - The folder **“instability/nohead/db\_Lsys”** contains instability study of two soft swimmers.
  - You can also find the comparison study of swimming speed before and after clustering in this folder. Please look at **“instability/nohead/vel/b12.0\_Lsys”** for the comparison study for swimmers without head.
  - Look at **“instability/withhead/b12.0\_Lsys”** for the comparison study for swimmers with head.
- The folder **“forces”** contains all the simulation scripts and data for the dynamic clustering study and clustering force measurements.
  - Please look at the folders **“forces/sdist/km100000/moving”** and **“forces/sdist/km100000/moving\_withhead”** for the dynamic clustering of two stiff swimmers.
  - Look at the folder **“forces/Lsys/moving/sdist10.0”** and **“forces/Lsys/moving/sdist10.0\_withhead”** for the dynamic clustering of two soft swimmers.
  - The folder **“forces/sdist/km400000”** contains the force measurement of two interacting stiff swimmers with vertical distance varying.
  - The folder **“forces/sdist/Dxs\_sdist3.2/”** contains the force measurement of two interacting stiff swimmers with horizontal distance varying.
  - The folder **“forces/Lsys”** contains the force measurement of two interacting soft swimmers with vertical distance varying.
  - The folder **“forces/Lsys/Dxs\_db0.0”** contains the force measurement of two interacting soft swimmers with horizontal distance varying.
  - The folder **“forces/Lsys/Ori”** contains the force measurement of two interacting soft swimmers with their orientation varying.
  - The folder **“forces/db4.0”** contains the force measurement of two interacting asymmetric stiff swimmers.
  - The folder **“forces/Lsys/Dxs”** contains the force measurement of two interacting asymmetric soft swimmers.

In all the folders mentioned above the files with name “in.run” are the input scripts for LAMMPS. The .data files are the data generated by the simulations. The python files are either preprocessing

or postprocessing scripts. To run these python scripts, the directory of the custom python module “pythonmod” has to be appended to the “PYTHONPATH” environment variable.

- The folder “**pythonmod**” contains the custom python modules needed for the preprocessing of the simulation model and postprocessing of the simulation output data.

**To generate the figures presented in the manuscript please run the following scripts:**

**Figure 2(a)**

single\_withouththead/vis/plotcomp.py

**Figure 2(b)**

single\_withouththead/vis/Length\_w0.8/plotcom.py

**Figure 3(a)**

single\_withouththead/mass/plotcom.py

**Figure 3(b)**

single\_withouththead/prescribing/prescribingwave1/plotw2.py

**Figure 4**

reciprocal/plotcom.py

**Figure 5(a) (b)**

forces/sdist/km100000/moving/plottrack2.py

inset: plotshapes.py

**Figure 6(a)**

forces/Lsys/moving/sdist10.0/plottrack.py

inset: plotshapes.py

**Figure 6(b) (c)**

forces/Lsys/moving/sdist10.0\_withhead/plottrack.py

(b) inset: plotshapes.py

(c) inset: plotshapes\_comp.py

**Figure 7(a) (b)**

instability/nohead/vel/b12.0\_Lsys/plot2com.py

inset:

instability/nohead/vel/b12.0\_Lsys/single\_w0.4/plotsnapshot.py

instability/nohead/vel/b12.0\_Lsys/pair\_w0.4/plotsnapshot.py

**Figure 7(c)**

instability/nohead/vel/b12.0\_Lsys/plotbinc\_p.py

**Figure 8 (a)**

instability/nohead/vel/b12.0\_Lsys/singlelevel/plotcom.py

**Figure 8 (b)**

instability/nohead/vel/b12.0\_Lsys/singlelevel\_L/plotcom.py

**Figure 9(a) (b)**

instability/withhead/b12.0\_Lsys/plot2com.py

inset:

instability/withhead/b12.0\_Lsys/single\_w0.4/plotsnapshot.py

instability/withhead/b12.0\_Lsys/pair\_w0.4/plotsnapshot.py

**Figure 10 (a)**

instability/nohead/db/db11.0625/plotshapes.py #set tau = 1.7

inset:

instability/nohead/db/db11.0625/plotsnapshot.py

**Figure 10 (b)**

instability/nohead/db/db11.0625/plotshapes.py #set tau = 3.0

**Figure 10 (c)**

instability/nohead/db\_Lsys/db1.65/plotshapes.py #set tau = 1

inset:

instability/nohead/db\_Lsys/db1.65/plotsnapshot.py

**Figure 10 (d)**

instability/nohead/db\_Lsys/db1.65/plotshapes.py #set tau = 2

**Figure 11 (a)**

instability/nohead/db/plotcom.py

**Figure 11 (b)**

instability/nohead/db\_Lsys/plotcom.py

**Figure 12 (a) (b)**

forces/sdist/km400000/plotf2.py

**Figure 12 (c) (d)**

forces/sdist/Dxs\_sdist3.2/plotfx.py

(b) inset: forces/sdist/Dxs\_sdist3.2/dxs4\_16/plotsnapshot.py

**Figure 13 (a) (b)**

forces/Lsys/plotf.py

**Figure 13 (c) (d)**

forces/Lsys/Dxs\_db0.0/plotfx2.py

**Figure 14**

forces/Lsys/Ori/plotf.py

inset:

forces/Lsys/Ori/phi-0.08/plotsnapshot.py

**Figure 15 (a) (b)**

forces/db4.0/Dxs/plotfx.py

(b) inset

forces/db4.0/Dxs/dxs4\_16/plotsnapshot.py

**Figure 16 (a) (b)**

forces/Lsys/Dxs/plotfx3.py

(b) inset

forces/Lsys/Dxs/dxs4\_16/plotsnapshot.py

**Figure 17(a)**

convergence/plotcomp.py

**Figure 17(b)**

convergence/prescribingwave/plotcomp.py