Simulating Spherical Ciliated Organism Locomotion: An AI-Driven Approach with DeepXDE

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Abstract

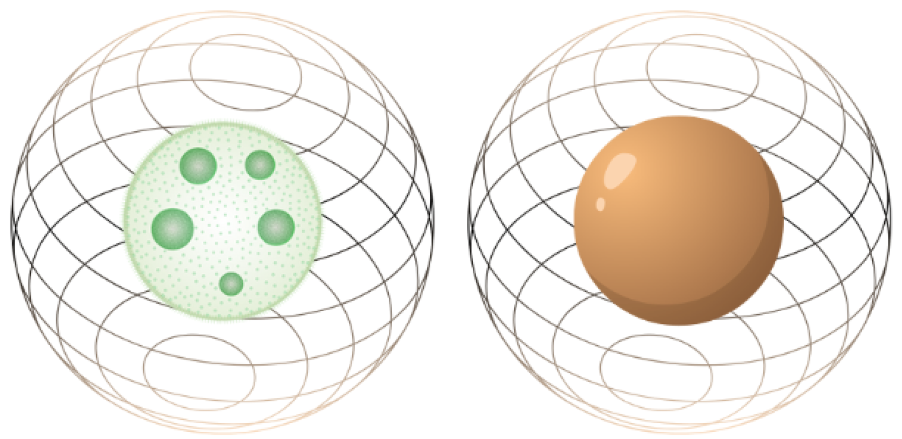
The study of microorganism propulsion has intrinsic relevance for the development of micro-robots designed for targeted drug delivery and as a foundation for further studies on hydrodynamic interactions of microorganisms in dense environments. Such a problem is governed by the Stokes equations, a system of partial differential equations (PDEs) describing fluid flow at low Reynolds numbers, where viscous forces dominate inertial forces. Recently, physics-informed neural networks (PINNs) have shown promise for approximating solutions to PDEs which govern physical laws. However, complex PDEs can be difficult to solve using PINNs and require increased computational costs. In comparison to analytical solutions, we evaluate the effectiveness of using PINNs to predict the propulsion of microorganisms. Our initial steps lead us to begin with the simpler case of characterizing the microorganism as a rigid sphere.

Acknowledgements

This research is supported by NSF grant DMS-2149865. We are very grateful to our mentors Dr. Nganguia and Dr. Yan, and program organizer Dr. Cornwell.

Introduction

- In our original problem, we want to use deep learning to verify the propulsion speed of a ciliated organism. We use the word, "verify", because the speed has already been proven to be 2/3 in dimensionless units.
- In our simplified problem, we set the propulsion speed for a rigid sphere to the constant 1.
- We will apply and optimize DeepXDE parameters, including activation functions and learning rates, to enhance the accuracy of these simulations.
- Once we enhance the accuracy of the program, we will move on to our original problem, a ciliated organism.



Ciliated Organism vs. Rigid Sphere

The Equations

The PDE

$\nabla p - \nabla^2 \vec{u} = 0$, Stokes Equation

$\nabla \cdot \vec{u} = 0$, Continuity Equation

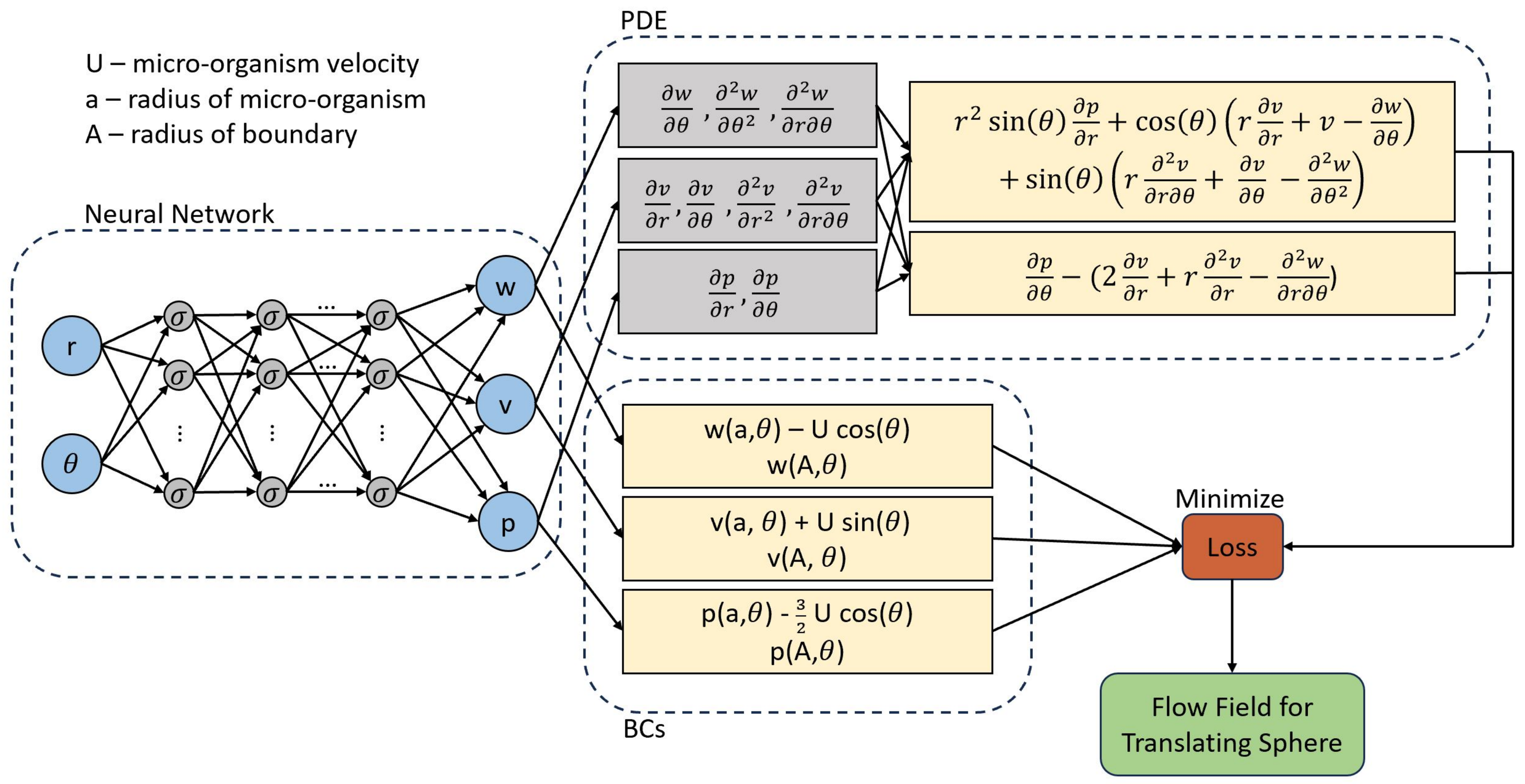
Boundary Conditions

$$u_r(r=1,\theta) = U\cos\theta$$
$$u_\theta(r=1,\theta) = -U\sin\theta$$
$$u_r(r\to\infty,\theta) \approx u_\theta(r\to\infty,\theta) \approx 0$$

Spherical Coordinates

$$\vec{u} = \langle u_r, u_\theta, u_\phi \rangle$$
$$u_x = u_r\cos\theta - r u_\theta \sin\theta$$
$$u_y = u_r\sin\theta + r u_\theta \cos\theta$$
$$|\vec{u}| = \sqrt{u_x^2 + u_y^2}$$

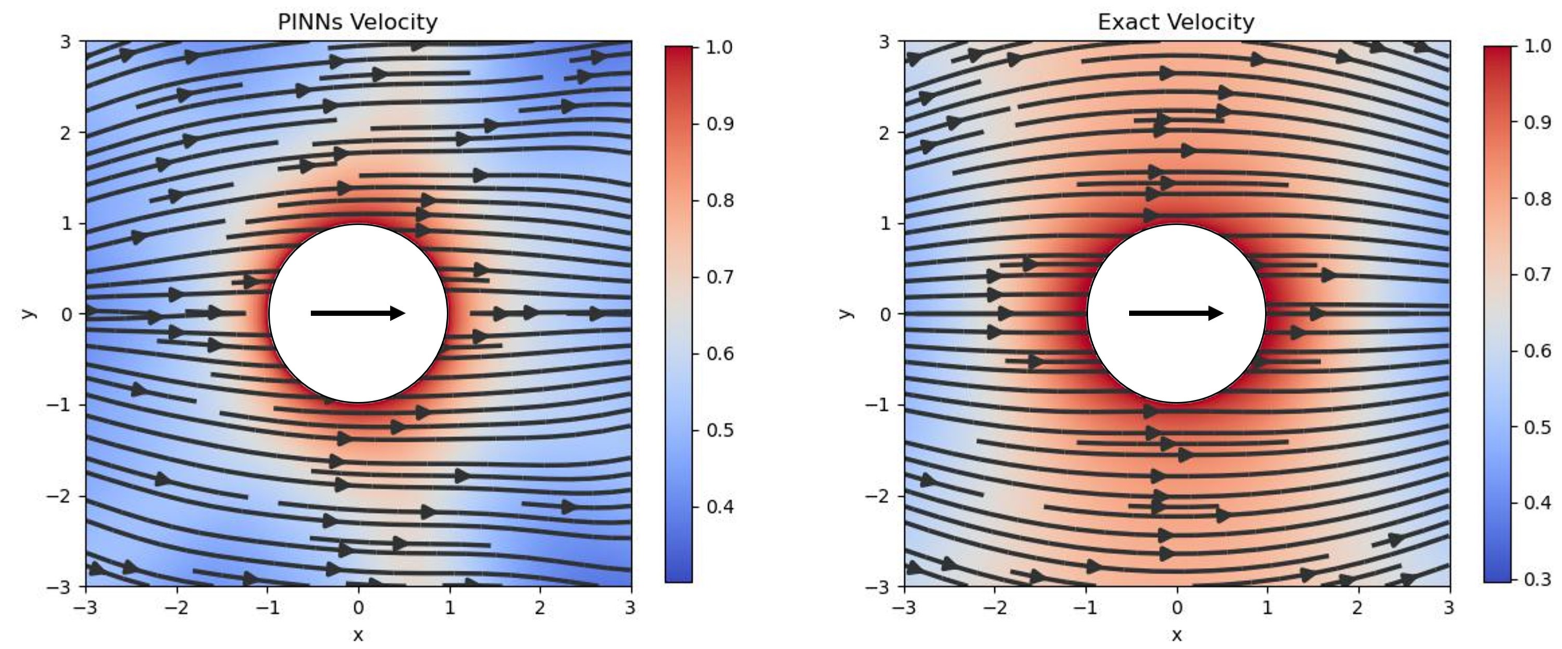
Physics-Informed Neural Networks (PINNS)



Our PINN...
($\mathrm{w} = u_r$, $\mathrm{v} = u_\theta$)

- Has inputs r and θ.
- Computes radial component w, tangential component v, and pressure p.
- Takes derivatives of w,v, and p and passes the values to our PDE.
- Accounts for values at the boundaries for w, v, and p.
- Minimizes loss to produce the flow field for a translating sphere.

Results



Comparison of flow field between PINN results and exact solution in Cartesian coordinates. The stream plot represents the direction of the fluid flow and the colormap represents the magnitude of $\vec{u}$.
L2 Errors: $\mathcal{E}_{u_r} \approx 0.2176, \mathcal{E}_{u_\theta} \approx 0.2093, \mathcal{E}_p \approx 0.0106$

Future Directions

To further our research, we will continue manipulating our code's hyper parameters to improve the accuracy of our simulations.
Once we achieve an exceptional error level, we will modify the code such that it represents a ciliated organism rather than a rigid sphere.

Further explorations of swimming microorganisms can lead to future advancements such as:

- Representation of future models consisting of unstable boundary conditions, compressible fluids, and multiple swimmers within a fluid.
- Demonstration of potential implications of our findings, particularly in the context of targeted drug delivery methods.

Bibliography

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