Identifying Symbolic Models for Particle-Laden Flows with Genetic Programming

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(1) Towards Improving Simulations of Flows around Spherical Particles Using Genetic Programming (CEC, 2022)

(2) Graph Networks as Inductive Bias for Genetic Programming: Symbolic Models for Particle-Laden Flows (evo*, 2023)

20th Humies Competition (2023) – Lisbon, Portugal

The approach in a nutshell

Numerical solvers are computationally

limited to $O(10^5)$ particles

→ Identification of symbolic closure models with Genetic Programming (GP)

- 1 particle
- 2 particles (Paper 1)
- *n* particles (Paper 2)

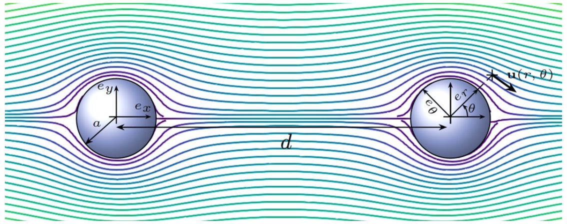
→ Requirements towards an equation:

- Accuracy
- Interpretability
- In-line with physical laws

→ We address a subdomain of the problem (Stokes flow, *Re* = 0)

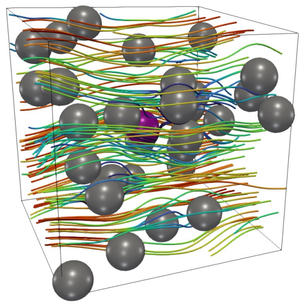
The approach in a nutshell

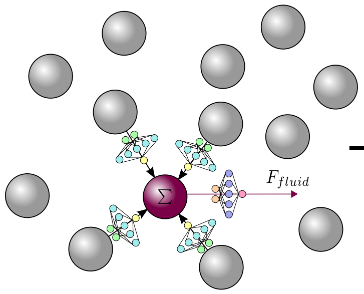
(1) GP is generally capable to identify physically meaningful models for the two-particle problem



$$u_d = u_\infty + a_0 u_0(x, y) + a_d u_d(x, y)$$

(2) GN as inductive bias facilitates to scale the problem to *n* particles





$$F_{fluid} = \sum_{i=0}^{n} a_0 \cdot (\sin(\theta) + a_1) \frac{1}{r}$$

Data from direct numerical simulation

Graph Network (GN) as inductive bias

Symbolic Model discovered by GP

Why is the result human-competitive?

The result is equal to or better than an result considered an achievement

in fluid mechanics at the time it was first discovered (F)

and is publishable on its own right (D).

Competing with past achievements

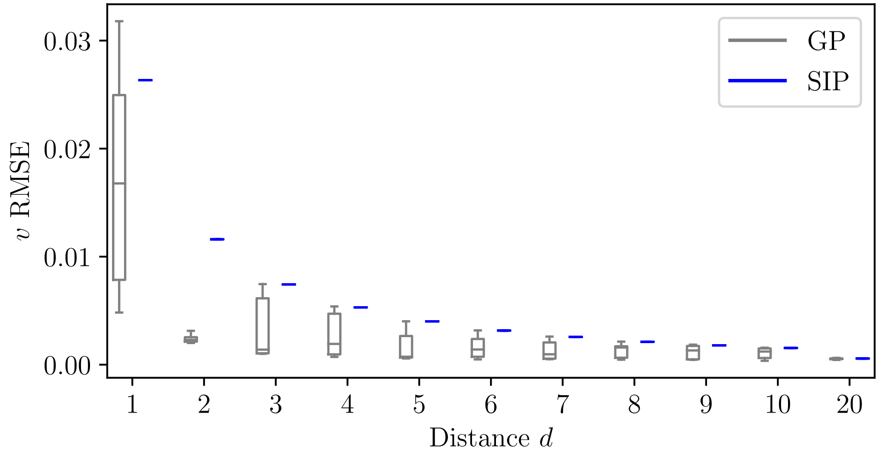
2 particles, paper (1)

- GP algorithm outperforms the super-imposition method (SIP)

***n* particles, Paper (2)**

- [3] introduces the pairwise interaction assumption in 2017
- In the Stokes regime, our equations are
  - on par with [3] in terms of accuracy
  - less complex than [3]

→ Both papers (1) and (2) present novel equations



Accuracy of equations for the two-particle problem, compared to SIP

Why is the result human-competitive?

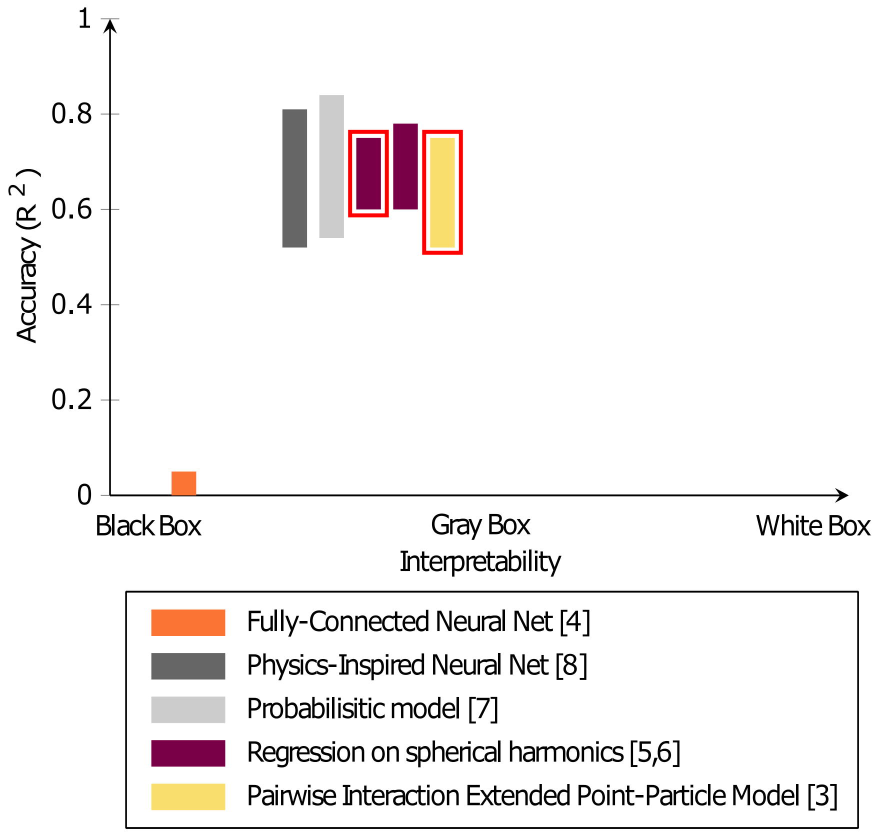
The result is equal to or better than the

most recent human-created solution for the Stokes flow,

for which there has been a succession of human-created solutions (E).

Our models fill the interpretability gap

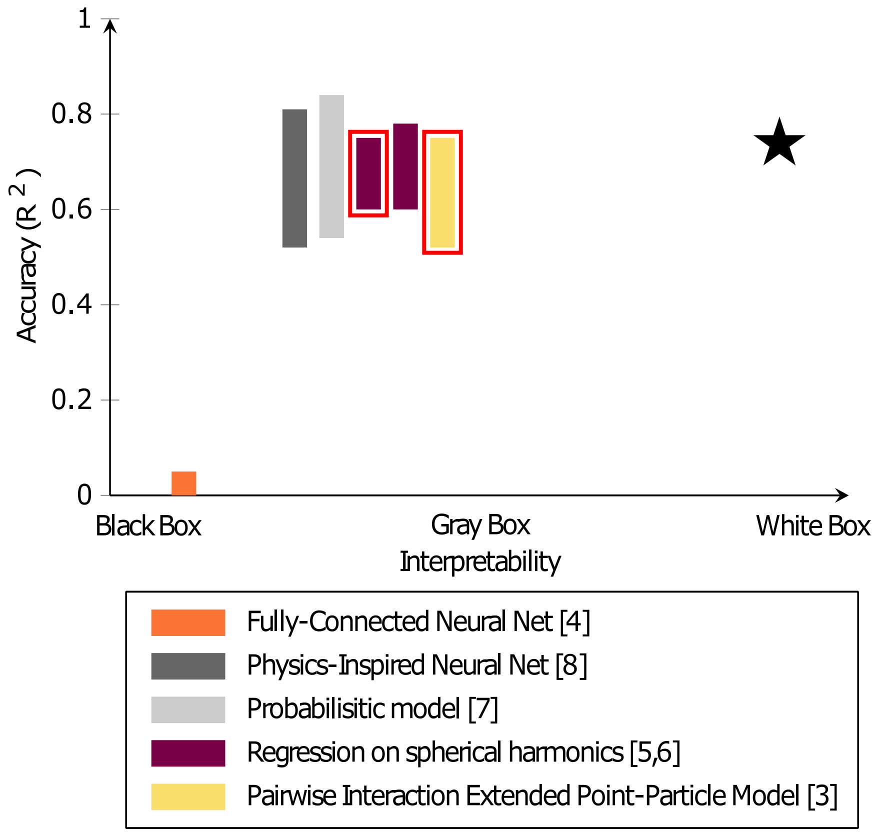
- Simulating particle-laden flows is one of the oldest problems in the history of fluid mechanics [1] (1933)
- Most recent iterations since 2017 to solve the problem:
  - Human-created correlations [3,5]
  - Data-driven models [4,6-8]



Our models fill the interpretability gap

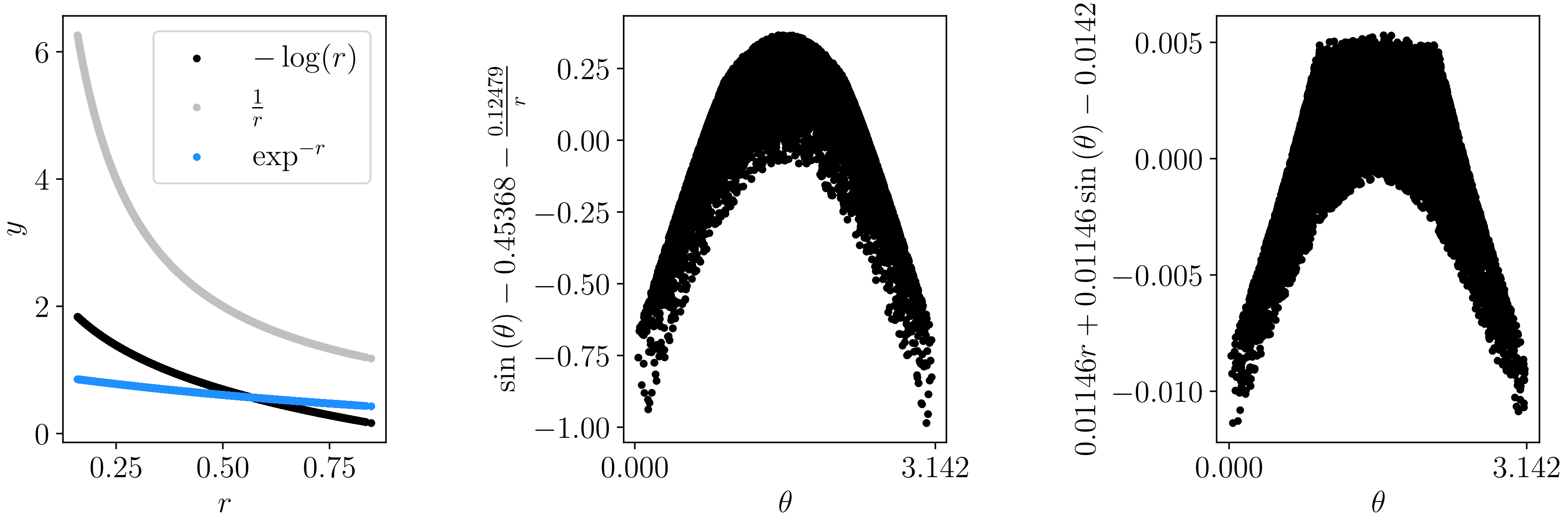
- Equations published in paper (2) achive similar accuracies as the SotA approaches, but are less complex

ϕ	Experiment	Equation	GP R^2
0.064	$y = g(x), c = 2$	$\sum\left(0.01146r + 0.01146\sin(\theta) - 0.0142\right)\frac{1}{r}$	0.798
	$y = g(x), c = 1$	$\sum\left((0.03448r + 0.03448\sin(\theta) - 0.04238)(-\log(r))\right)$	0.820
	$y = f(g(x))$	$0.0992\sum\left((r(\sin(\theta) - 0.1312) - 0.1983)(-\log(r))\right) + \bar{u}_x^f - 0.3177$	0.864
0.125	$y = g(x), c = 2$	$\sum\left(0.01397\sin(r) + 0.01397\sin(\theta) - 0.01724\right)\frac{1}{r}$	0.778
	$y = g(x), c = 1$	$\sum\left(0.00839 + (0.01578\sin(\theta) - 0.01644)\frac{1}{r}\right)$	0.792
	$y = f(g(x))$	$0.0597\sum\left(\left(\sin(\theta) - 0.45368 - \frac{0.12479}{r}\right)e^{-r}\right) - 0.0616$	0.822
0.216	$y = g(x), c = 2$	$\sum\bar{u}_x^f\left(\sin(\theta) - 0.57328 - \frac{0.10557}{r}\right)$	0.720
	$y = g(x), c = 1$	$\sum\left(0.00944 + (0.01932\sin(\theta) - 0.01982)\frac{1}{r}\right)$	0.797
	$y = f(g(x))$	$0.1166\sum\left(\left(0.17448\sin(\theta) - 0.08318 - \frac{0.01419}{r}\right)\frac{1}{r}\right) - 0.1602$	0.793
0.343	$y = g(x), c = 2$	$\sum\left((0.08249\sin(\theta) - 0.07348)(-\log(r)) + 0.00539\right)$	0.791
	$y = g(x), c = 1$	$\sum\left((0.08749\sin(\theta) - 0.07348)(-\log(r)) + 0.00423\right)$	0.792
	$y = f(g(x))$	$0.3904\sum\left(\left(0.10982e^{\sin(\theta)} - 0.26635\right)(-\log(r)) + 0.0165\right) - 0.0421$	0.808



What makes our entry special?

- Equations help to gain insights into the underlying particle interactions.
- Identified building blocks are a promising starting point to approach more complex flow regimes.

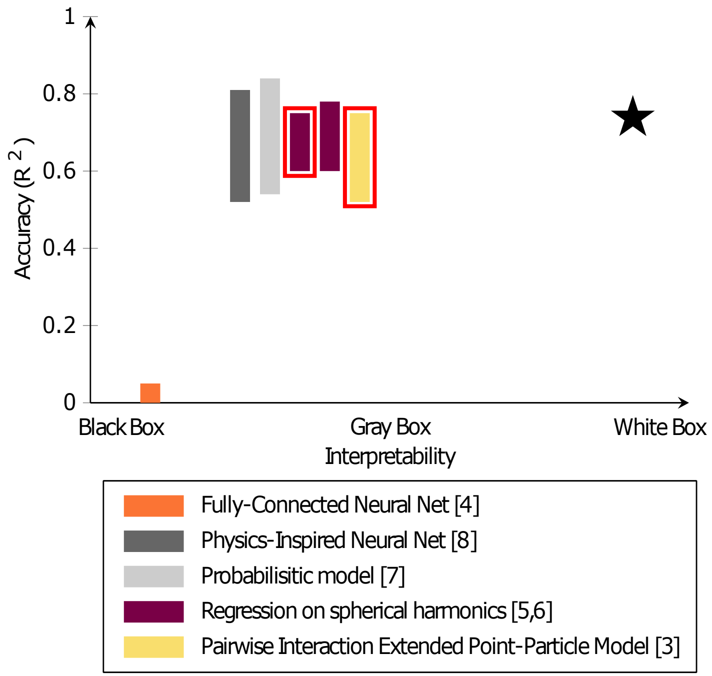


Paper (2): Plots of frequently appearing building blocks in the symbolic models

What makes our entry special?

- High requirements:
  - Accuracy
  - Interpretability
  - In-line with physical laws

} Strong constraints on the algorithms



- Initially, the success of GP was strongly doubted
- Within the Stokes regime, our equations from (2) are not only human-competitive, but also ML-competitive

Literature

[1] L. Schiller, and A. Maumann. "Über die grundlegenden Berechnungen bei der Schwerkraftaufbereitung". In: Zeitschrift des Vereines deutscher Ingenieure 77 (12): 318--320 (March 1933)

[2] G. Akiki, T. L. Jackson, and S. Balachandar. "Force variation within arrays of monodisperse spherical particles". In: Phys. Rev. Fluids 1, 044202 (August 2016).

[3] G. Akiki, T. L. Jackson, and S. Balachandar. "Pairwise interaction extended point-particle model for a random array of monodisperse spheres". In: Journal of Fluid Mechanics 813 (Feb. 2017), pp. 882–928.

[4] S. Balachandar et al. "Toward particle-resolved accuracy in Euler-Lagrange simulations of multiphase flow using machine learning and pairwise interaction extended point-particle (PIEP) approximation". In: Theoretical and Computational Fluid Dynamics 34.4 (Aug. 2020), pp. 401–428.

[5] W. C. Moore and S. Balachandar. "Lagrangian investigation of pseudo-turbulence in multiphase flow using superposable wakes". In: Physical Review Fluids 4.11 (Nov. 2019), p. 114301.

[6] W. C. Moore, S. Balachandar, and G. Akiki. "A hybrid point-particle force model that combines physical and data-driven approaches". In: Journal of Computational Physics 385 (May 2019), pp. 187–208.

[7] A. Seyed-Ahmadi and A. Wachs. "Microstructure-informed probability-driven point-particle model for hydrodynamic forces and torques in particle-laden flows". In: Journal of Fluid Mechanics 900 (Oct. 2020), A21.

[8] A. Seyed-Ahmadi and A. Wachs. "Physics-inspired architecture for neural network modeling of forces and torques in particle-laden flows". In: Computers & Fluids 238 (Apr. 2022), p. 105379.

[9] B. Siddani, S. Balachandar. "Point-particle drag, lift, and torque closure models using machine learning: Hierarchical approach and interpretability". In: Physical Review Fluids 8 (2023).

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THANK YOU FOR YOUR ATTENTION!

Code for paper (2):

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