Physics Informed Neural Networks for efficient modeling of concentrated suspension flows

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Microstructure and flow behavior of moderate to high concentration suspensions of rigid particles are topics of considerable scientific significance given the large amount of diverse technological applications like painting, coatings, composite structures, drugs and food to name a few.
The modeling and simulation of such systems is extremely challenging and requires advanced numerical methods like massively parallel Finite Element simulation in order to deal with specific bottlenecks arising in this context.
Some of these are : remeshing due to the continuous particle position and orientation evolution, collision detection and contact forces calculation. In addition to these, the problem can only be solved for a small representative volume and then the results can be extended to the macroscopic scale of the physical system by means of upscaling or numerical homogeneization techniques.
As of today, the complete problem is practically untreatable by direct simulation even using high performance computing. Even using parametric model order reduction techniques, the computation remains burdensome if not nearly impossible, since concentrated suspensions have a significant amount of configurational degrees of freedoms resulting in an exponentially growing computational complexity. Hence the problem is classically addressed by using approximate models to describe the kinetics and the interactions at the particle scale and that are upscaled using a statistical approach. These approaches are only satisfactory for simple particle geometries and suspending fluid behaviors.
In the last four years, Physics Informed Neural Networks (PINN) have emerged as a technique to solve complex physics through the use of artificial intelligence. Indeed, neural networks have been shown to be able to predict the behavior of a physical system described by a set of partial differential equations. The advantages of using this method are numerous. First, the method is not mesh based and does not require remeshing as the as in Finite Element methods. Moreover, through automatic differentiation, it is possible to estimate derivatives exactly to machine precision hence suppressing the discretization error. Most importantly PINNs can integrate data both from other numerical simulations and experiments and notably they can accept whole 3D images as inputs therefore avoiding the complex task of parametrizing the system configuration.
PINNs are rapidly spreading throughout the scientific community of computational solid and fluid mechanics and showing promising results for the fields where they are already been applied.

This thesis work would be the first attempt of artificial intelligence at solving complex rheology. Using the ICI-tech libraries that are already available at our laboratory, we can generate realistic 3D images of concentrated solutions with given configurations. These images can be used to train PINN in order to predict the flow and particles configuration in moderately to highly concentrate suspensions, therefore learning the suspension rheology solely from the knowledge of the properties of its constituents.