A web-based cloud platform for high-resolution jet break-up analysis of Newtonian and non-Newtonian fluids

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In this work we aim to develop a platform with open-source tools for solving the injection of Newtonian and non-Newtonian fluids into another medium with high-resolution computational techniques. Currently, the discipline is being driven by expert users with low adoption among experienced domain professionals. Offering computational fluid dynamics (CFD) tools to the latter group with easy-to-use interfaces implemented with cutting-edge techniques and connected to remote high-performance/cloud computing will open a way to new innovative products. Although multiple commercial and non-commercial solutions are available on the market, not many efforts have been made to provide open-source frameworks with the characteristics described above.

In particular, we focus our attention on a common problem where size distributions play a key role, as for example the injection of one fluid into another. Examples of industrial processes are chemical mixing, aeration, 3D printing, pharmaceutical application or agricultural pesticide disposal. These applications require precise drop or bubble sizes for process optimization, safety evaluation or health care regulations. In order to meet these requirements, the proposed CFD framework includes the capability of obtaining high-resolution data for Newtonian and non-Newtonian fluids.

This framework is based on cloud technologies, namely HPCCloud (v2.0.0), a novel open-source web-based simulation environment platform developed by Kitware. In this work, using the HPCCloud stack, we propose the implementation of a new workflow and functionalities enhancing and facilitating the use of CFD tools for this specific application. The following items summarize the main contributions:

- CFD model: parametrizable orifice and planar jets models based on the OpenFOAM volume of fluid method (interIsoFOAM, v1806). The model has been validated with state-of-the-art experiments for different regimes, such as dripping, varicose, sinuous and atomization. Implicit large eddy simulations with different grid resolutions up to 1 billion cells (10 µm cell size) have been performed for the validation in order to analyze the effects of the turbulence in the break-up.
- Post-processing: a new in-house VTK-based program for automatically computing and visualizing the drop size from the cells volume fraction.

- Computing: in addition to the existing remote connection to traditional high-performance computing servers or Amazon Web Services (AWS), we extended the integration of cloud computing, for instance IBM Cloud™ Private, for providing pre-configured tools ready to use with data privacy.
- Front-end: the improvements described above have been included in the HPCCloud front-end, in addition to a customized visualization stage for rendering results and size distributions.

The development of this tool will provide researchers and engineers with the capability of easily investigating the break-up complex problems based on high-resolution computational fluid dynamics, but also is a proof-of-concept for an open-source simulation framework built with modern web-technologies.