Towards the development of high performance scientific software for simulating 3D fluid-dynamic processes in a viscoelastic fluid

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To understand the onset and the evolution of rheological behavior of materials realized by adding solid fillers to viscoelastic fluids, a collaboration between computing scientists and chemical engineers was established to develop scientific software to simulate such processes on high end computing infrastructures. The results of this activity will be used as starting point of future applications in industrial processes such as flow intubation and injection molding.

The specific application that we consider consists of a single sphere in a sheared viscoelastic fluid. Assuming incompressibility, negligible inertia, and buoyancy free conditions the governing equations are the continuity (mass balance) and momentum balance equations, plus a constitutive equation depending on the nature of the suspending liquid [2].

Governing equations (non linear evolutionary PDEs) are discretized by using finite elements, while linearization is based on a semi implicit scheme which gives rise to a linear systems to solve at evolution step whose matrices are large (i.e. $O(10^6)$ unknowns), symmetric and sparse.

Taking into account that the underlying mathematical model is described by partial differential equations and to guarantee code *maintainability, portability, reusability and efficiency*, the parallel computing environment that supports the simulation software relies on PETSc (Portable, Extensible Toolkit for Scientific Computation) components [1] integrated with the TFEM (Toolkit for Finite Element Method) software toolkit [3], already employed to discretize and solve 2D problems.

We discuss computational efforts towards the development of high performance software tools needed to perform such computational expensive simulations. We also address the *validation* of numerical results and *performance* gain on the basis of same case studies.

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