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# MODELING OF MULTIPHASE FLOWS USING A HIGH ORDER PARALLEL FINITE ELEMENT METHOD

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**Summary:** *Our work concerns multiphase flows and, in particular, modeling of the rubber mixing processes. For that, we use an adaptive finite element solver, developed to meet good results accuracy. Within this framework, an implicit boundary approach describes the phases interface evolution. Based on a distance computation method (level-set), we deal with complex geometries and run linear as well as non-linear material simulations, all optimized to give highly accurate results with optimized computation time. In this paper, we present high order stabilized finite elements implemented in ICI-Tech, our scientific computing library, their performances, and parallel efficiency for classical advection and diffusion problems.*

## 1 INTRODUCTION

Several industrial contexts employ mixing processes, in food, polymer, or pharmaceutical domains. Several types of mixers exist, such as two-roll mills, continuous mixers, and internal batch mixers[1]. Simulation is today a powerful tool for process design, from the laboratory to the industry scales. This work is part of a more global project which concerns building an efficient numerical tool to model rubber behavior evolution in an internal mixer, based on ICI-tech, a scientific computing library developed at ICI (the High Performance Computing Institute) [2] and using open source libraries, such as PETSc [3] and MFEM [4]. For that, we first detail the implementation of a parallel high order finite element method used to solve the convection-diffusion equation (and find numerical solutions for the heat transfer problem, for example). Then, we extend the challenge to highly convective situations and apply it to the interface capture problem (necessary to distinguish the different phases – like rubber, air, or mixer – in the computational domain). Resolution of Laplace's equation tests the developed solver for a steady-state configuration, by computing L2 and H1 errors for different interpolation orders, using the analytical solution. For transient convection problems, the implementation of a high-order time solver allows to keep the balance between both spatial and time errors. Finally, the high order method proves to be efficient within the parallel framework of ICI-tech, necessary for large scale simulations.

## 2 LEVEL SET USING HIGH ORDER FEM

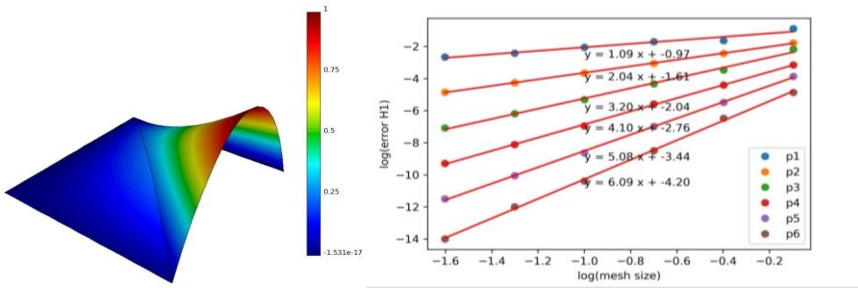
The main advantage of coupling the level set method and the FEM is that it allows for more simplicity and accuracy in the handling of the geometry of the computational domains, in particular for multiphase problems. Even though it is common to use the lowest order continuous finite element approximation for this type of coupling, we have developed various higher-order approximations and found a good compromise between accuracy and computational costs, when validating the C++ code implemented in ICI-Tech by running an error H1 study: first for Laplace's equation by using an analytical solution and second for convection by using a very high order calculated level set solution. The Laplace's equation is written as follows, where the problem is: find *u(x)* such that:

$$\begin{cases} -K\Delta u = f & u \in \Omega \\ u = u_0 & u \in \partial\Omega \end{cases} \tag{1}$$

Where $\Omega$ is the computational domain, $K$ is the diffusion coefficient and $f$ is the source term. The following logarithmic graphs show the computed error H1 according to the variation of the mesh size on a 2D unit square where boundary conditions are: *u(x)=sin(x)* on the top side and 0 elsewhere on the boundary. The analytical solution of equation (1) is:

$$u(x,y) = \frac{1}{sinh(\pi)} sin(\pi x)\, sin\, h(\pi y) \tag{2}$$

Figure 1 shows the convergence curves, through the plot of the H1-error, for second, third, and fourth-order interpolations. It shows that the H1-norm error decreases at the rate of *n*, the interpolation order. It also clearly shows that the convergence rates are of order $O(h^n)$ for $n$ = 1, 2, 3, 4, 5, 6 as theoretically predicted in [2].




(a) (b)

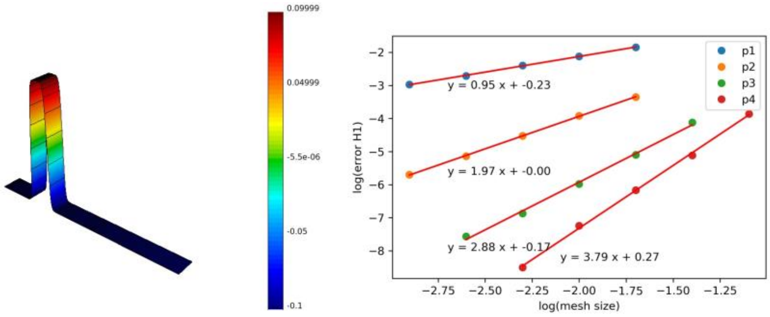
Figure 1 – (a) Numerical results computed with 2 elements of order P2. (b) Error H1 as a function of the mesh size (from 0.025 (2000 elements) to 0.8(2elements)) for different interpolation orders

## 2 CONVECTION OF LEVEL SET USING A HIGH-ORDER TIME SOLVER

The convection equation generally writes as follows, where the problem is: find *u(x,t)* such that:

$$\begin{cases} \frac{\partial u}{\partial t} + v\nabla u = f & u \in \Omega \\ u(x,0) = u_0 \end{cases} \tag{3}$$

being $v$ the flow velocity. To avoid having too short time steps that lead to higher computational times, the time scheme should be equivalent to the spatial one, where the overall error will be equally dependent on spatial and time error. It is possible to do so by using a high-order time scheme. To gain in accuracy, one uses: a backward Euler method for time interpolation with the first-order space scheme; the Crank-Nicolson time discretization [7] for the spatial second-order; the Rosenbrock method [8] in time for P3 and P4 in space. Figure 2-(a) shows the geometrical representation of a wave of a length equal to 1 immersed into a rectangle of a length equal to 10. Advecting the wave with a velocity 1 we obtain the corresponding H1 error plot variates according to the mesh size from 0.0025 to 0.08 for the interpolation orders P1, P2, P3 and P4 and is shown in Figure 2-(b). The convergence rates of the error are also of order $O(h^n)$ for $n = 1, 2, 3, 4$, same as for diffusion.

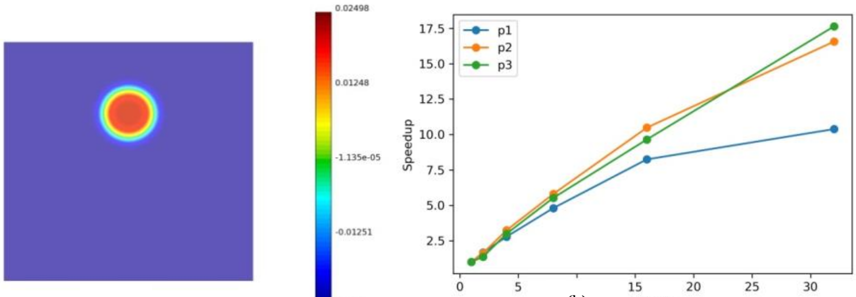



(a) (b)

Figure 2 – (a) Numerical results computed with elements of order P1. (b) Error H1 as a function of the mesh size for different interpolation orders.

## 3 HIGH ORDER AND PARALLEL COMPUTATION

The parallel framework inherent to ICI-tech integrates all the high-order developments. A speedup test is performed to show the feasibility, but also the advantage of using high-order elements in parallel. Hence, we consider a a circle of a 0.7 radius in a unit-square domain, represented using a level-set approach [5], where the mesh size is 0.01. We then advect the circle using a rotating velocity field for 2 seconds and solve the convection problem with first, second and third-order interpolations of the solution. In Figure 3-(a), we observe the initial level-set representing the circle, and the speed-up curves are shown in Figure 3-(b). For the same mesh size, acceleration is better for P2 and P3 than P1. Also, one expects that, above a certain number of used cores, the parallel computation is still feasible for P2 and P3, while for P1 it is not.




(a) (b)

Figure 3 – (a) Immersed circle represented by Level-set function. (b) Speedup curves (speedup=t_one core/t)

## 4 CONCLUSION

In this work, a high-order finite element method is implemented in a parallel scientific computing library, ICI-Tech. An error test using an analytical solution is done for a 2D diffusion and 1D convection problem showing how the error convergence rate matches the interpolation order, thus showing the advantages of using high-order schemes regarding result accuracy. Finally, a speedup test is performed to show the advantage of using high order method in parallel computation.

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