Evaluation of CFD codes on a two-phase flow benchmark reference test case

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***Abstract*—The performance of two commercial simulation codes, Ansys Fluent and Comsol Multiphysics, is thoroughly examined for a recently established two-phase flow benchmark test case. In addition, the commercial codes are directly compared with the newly developed academic code, FeatFlow TP2D. The results from this study show that the commercial codes, failing to converge and produce accurate results, leave much to be desired with respect to direct numerical simulation of flows with free interfaces. The academic code on the other hand was computationally efficient, produced very accurate results, and outperformed the commercial codes by a magnitude or more.**

I. Introduction

Commercial software tools are widely used by industrial engineers today to simulate various physical processes. Except for cost, they offer many benefits over academic tools; commercial codes are reasonably easy to use, are often documented extensively, have user support, and usually produce qualitatively good results. However, what is not known is how accurate these codes really are, on an absolute level, and what performance can be expected for a specific problem. This was, within the context of two-phase flows, examined by simulating a recently established benchmark test case with two different commercial codes, the general and flexible simulation package Comsol Multiphysics and the dedicated computational fluid dynamics (CFD) flow solver Ansys Fluent. The results from these codes were also compared with those computed with a newly developed academic code, FeatFlow TP2D [4]. The test problem was chosen to examine the codes abilities to accurately simulate two-phase fluid flows with immersed interfaces, and consisted of tracking the evolution of a bubble rising and deforming in a liquid column [5]. For this numerical benchmark test case an accurate reference solution has been established [6] which enabled quantitative validation and comparison of the codes.

II. Commercial software tools

This section explores the accuracy and performance of the two commercial codes, Comsol Multiphysics and Ansys Fluent, for simulating the chosen benchmark test problem.

A. Comsol Multiphysics

The Comsol Multiphysics software suite (previously marketed under the name Femlab) is a finite element package for solving coupled systems of partial differential equations (PDEs). Although the software is very user friendly, has a nice graphical user interface, and allows for almost arbitrary PDE based problems to be postulated, the monolithic fully coupled approach and heavy dependence on direct solvers limits its practical use to rather small problem sizes. Despite this, Comsol Multiphysics was applied to the benchmark test case in order to establish what a general commercial simulation tool, not optimized for CFD problems, can accomplish.

TABLE I
Simulation statistics and timings for Comsol Multiphysics

$1/h$	NEL	NDOF	NTS	MEM	CPU
20	800	13163	277	175	101
40	3200	51923	115	446	483
60	7600	116283	120	890	986
80	12800	206243	120	1568	2361

The following simulations were performed with version 3.3a of Comsol Multiphysics coupled with the conservative level set application mode which is used to model two-phase flow phenomena. A purely Cartesian tensor product grid was employed in the calculations with continuous biquadratic and discontinuous linear finite element basis functions, the Q_2P_1 Stokes elements, discretizing the velocity and pressure. The level set field was correspondingly discretized with conforming Q_2 basis functions.

All the following computations (including those of Fluent and TP2D for comparison purposes) were performed on a server with a 2.0 GHz Intel Core2Duo processor for which simulation statistics are given in Table I. The first column $1/h$ shows the reciprocal of the cell size which is equal to the number of cells resolving the width of the computational domain. The total number of cells or elements is denoted by NEL, the number of degrees of freedom by NDOF, and the number of time steps by NTS. The computational effort required can be seen from the peak memory consumption in Megabytes (MEM) and the required time to complete the simulations (CPU).

Although a comprehensive selection of iterative linear solvers is included in Comsol Multiphysics, the default and most robust choice is to use a direct solver. The magnitude of the peak memory consumption, although scaling linearly with the number of degrees of freedom, was very high due to the fully coupled approach. It was in fact impossible to obtain a solution for anything larger than a 80×160 grid, even when switching to the iterative solvers, which either failed to converge or still allocated too much memory. The variable

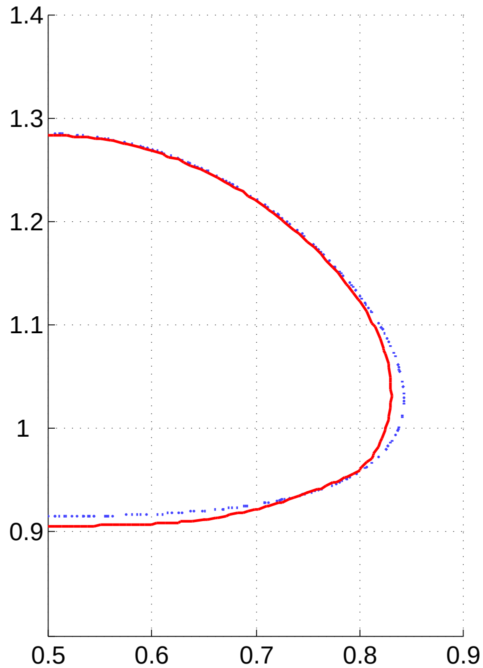

Fig. 1. Bubble shape computed with Comsol Multiphysics on the finest 80×160 grid (solid red), compared with the reference solution (dashed blue)

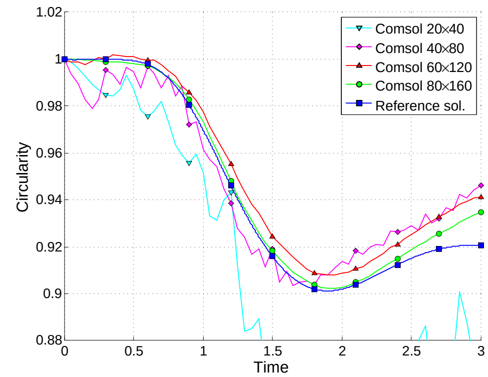

Fig. 2. Computed circularity curves for Comsol Multiphysics

TABLE II

MINIMUM CIRCULARITY WITH CORRESPONDING INCIDENCE TIME, AND ERRORS FOR COMSOL ($Ref.$ INDICATES REFERENCE VALUES)

$1/h$	$\not{c}_{min}$	$t\vert_{\not{c}=\not{c}_{min}}$	$\vert e_{\not{c}}\vert$
20	0.8402	2.25	$3.6{\cdot}10^{-2}$
40	0.9034	1.65	$1.0{\cdot}10^{-2}$
60	0.9081	1.90	$8.0{\cdot}10^{-3}$
80	0.9022	1.95	$2.9{\cdot}10^{-3}$
$Ref.$	0.9012	1.90	

order DASPK time stepping scheme on the other hand worked very well, only requiring about 120 time steps to complete each simulation for all but the coarsest grid.

The bubble shapes at the final time ($t = 3$) computed on the finest 80×160 grid can be seen in Fig. 1. The results look quite good and believable in the picture norm although the computed bubble shape exhibit slightly more rounded contours than the reference solution.

The use of the reference benchmark quantities defined in [5] makes it easier to spot convergence trends, therefore the computed circularity, $\not{c}$, which is a measure of shape deformation, is compared against the established reference curve (Fig. 2). The results for the two coarsest grids, 20×80 and 40×80, show very oscillatory behaviors for which the means deviate significantly from the reference curve. The curves corresponding to the two finer grids behave better but increase towards the end of the simulation (after $t = 2.5$) instead of converging to a stable shape indicated by the blue reference solution.

Table II shows the minimum circularity, $\not{c}_{min}$, with corresponding incidence times, $t|_{\not{c}=\not{c}_{min}}$, and also the time averaged relative error of the circularity, $|e_{\not{c}}|$. Except for the very coarsest grid, the minimum circularity is quite close to the reference value, with an error of $1.0{\cdot}10^{-3}$ on the finest grid. The corresponding incidence times fluctuate somewhat and one would ideally like to have more data for finer grid levels to really be able to establish a convergence trend. The time averaged relative error is three times larger than that of the minimum on the finest grid, due to the diverging behavior after $t = 2.5$.

These tests have shown that although the Comsol Multiphysics package actually can simulate two-phase flows some real difficulties do exist. Firstly, the results do not seem to converge towards the correct solution for longer time periods, and secondly the approach used to solve and invert the discretized matrices consumed far too much memory to be able to run simulations with even moderately dense grids.

B. Ansys Fluent

The CFD package Ansys Fluent has been marketed as ”the world leader in Computational Fluid Dynamics” [1] and ”a state-of-the-art computer program for modeling fluid flow” [2], and thus has a lot to live up to. Fluent includes a comprehensive set of models to treat various flow related phenomena such as heat transfer, turbulence, combustion, chemical reactions, and also multiphase flows. Flows with immiscible fluids are treated with the Eulerian volume of fluid (VOF) methodology which employs the use of a scalar volume fraction function indicating the relative amounts of the fluids present in each computational cell.

Fluent employs a finite volume discretization in space with unknowns located at the cell centers. In the time domain there are a number of discretization schemes to choose from, of which the recommended implicit Fractional step operator spitting scheme has been used in the following tests. This scheme, which is a form of projection method, effectively separates the solution of the pressure from the velocity calculations, thus saving computational effort. To solve the arising linear equation systems Fluent employs an algebraic multigrid approach. In the following, version 6.3 of Ansys Fluent is used

TABLE III
SIMULATION STATISTICS AND TIMINGS FOR ANSYS FLUENT

$1/h$	NEL	NDOF	NTS	MEM	CPU
40	3200	12800	150	96	45
80	12800	51200	480	111	254
160	51200	204800	1200	210	2106
320	204800	819200	3000	439	21091

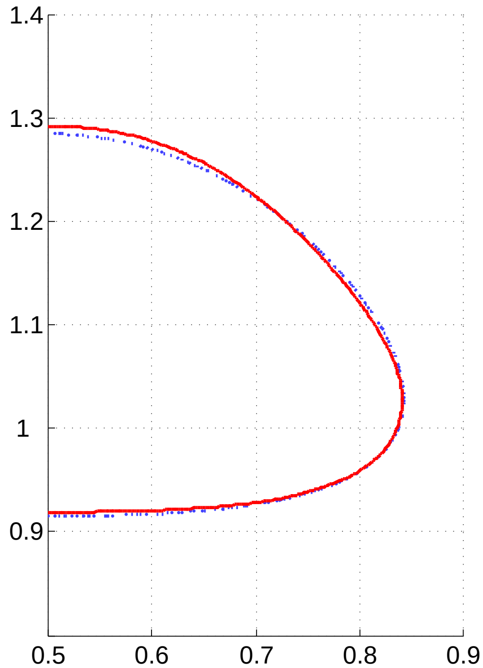

Fig. 3. Bubble shape computed with Fluent on the finest 320×640 grid (solid red), compared with the reference solution (dashed blue)

to perform benchmark tests identical to the ones previously done with Comsol Multiphysics.

The simulation statistics and timings for Fluent can be seen in Table III. Compared to Comsol Multiphysics, Fluent allocated significantly less memory and allowed the use of finer grids. However, it should be pointed out that since Fluent uses cell centered degrees of freedom the total number of unknowns is four times fewer than used by the Comsol software for a grid of the same size (Comsol Multiphysics also allows for higher accuracy with the employed Q_2 finite element discretization). The time steps were selected so that the capillary time step restriction was respected. Although the calculations for a given grid consumed less CPU time than for Comsol Multiphysics, it can not say anything about the level of accuracy achieved.

Computations on very coarse grids produced bubble shapes which deviated significantly from the reference solution. Refining the grids allowed the simulations to converge towards the reference shape, which is evident from Fig. 3, which shows the bubble shape at time $t = 3$ computed on the finest 320×640 grid. It is in fact quite hard to see any significant differences between the computed and reference solutions.

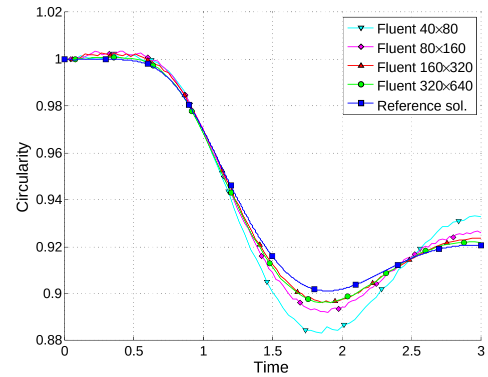

Fig. 4. Computed circularity curves for Ansys Fluent

TABLE IV
MINIMUM CIRCULARITY WITH CORRESPONDING INCIDENCE TIME, AND ERRORS FOR FLUENT ($Ref.$ INDICATES REFERENCE VALUES)

$1/h$	$\not{c}_{min}$	$t\vert_{\not{c}=\not{c}_{min}}$	$\vert e_{\not{c}}\vert$
40	0.8834	1.86	$8.2{\cdot}10^{-3}$
80	0.8922	1.90	$4.3{\cdot}10^{-3}$
160	0.8962	1.92	$2.4{\cdot}10^{-3}$
320	0.8963	1.92	$2.3{\cdot}10^{-3}$
$Ref.$	0.9012	1.90	

Since the final shape was quite accurate one might expect that the overall temporal evolution also is correct. However, if one looks at the curves for the circularity (Fig. 4) one can see that this actually is not the case. Although mesh independent solutions are obtained with the two finest grids, they do not converge towards the reference solution. It is apparently a period around the maximum deformation, between $t = 1.2$ and $t = 2.5$ (corresponding to the point of minimum circularity), that causes the most difficulties for Fluent.

The maximum errors and also the time averaged errors of the circularity are quite large as can be seen from Table IV. The values from the two finest grids show that a mesh independent solution has indeed been obtained. However, this solution does not converge towards the reference solution. The minimum circularity is predicted to occur slightly too late with a smaller value than expected. Comparing these errors with those produced by Comsol Multiphysics (Table II) one can see that both codes achieve quite similar levels of accuracy. Fluent has a slight advantage in the averaged error norm while Comsol produces better values for the minimum circularity.

III. ACADEMIC SOFTWARE TOOLS

Academic software tools often utilize the newest and most experimental algorithms in contrast to commercial tools which mostly apply tried and tested routines. It is therefore interesting to see if there exist any performance differences between a newly developed academic code and what commercial software can offer.

The benchmark test case used previously is therefore also used to measure the performance of an academic two-phase flow code, Featflow TP2D.

TABLE V
SIMULATION STATISTICS AND TIMINGS FOR FEATFLOW TP2D

$1/h$	NEL	NDOF	NTS	MEM	CPU
40	3200	19561	150	15	15
80	12800	77521	450	55	185
160	51200	308641	1000	212	1674

TABLE VI
MINIMUM CIRCULARITY WITH CORRESPONDING INCIDENCE TIME, AND ERRORS FOR TP2D ($Ref.$ INDICATES REFERENCE VALUES)

$1/h$	$\not{c}_{min}$	$t\|_{\not{c}=\not{c}_{min}}$	$\|e_{\not{c}}\|$
40	0.9002	1.88	$7.2{\cdot}10^{-4}$
80	0.9007	1.88	$2.8{\cdot}10^{-4}$
160	0.9010	1.91	$1.9{\cdot}10^{-4}$
$Ref.$	0.9012	1.90	

A. FeatFlow TP2D

The FeatFlow TP2D code is a new approach to simulate immiscible fluid flows which essentially consists of combining a non-conforming finite element flow solver with a conforming level set interface tracking method, and incorporating the surface tension forces semi-implicitly [3]. This technique, although somewhat unconventional, has resulted in a simulation code which has proved to be able to simulate two-phase flows with free interfaces both accurately and efficiently [4].

The simulation statistics and timings for TP2D are shown in Table V. Compared to the commercial codes, the required CPU time was notably smaller with respect to both grid size and the number of degrees of freedom (compare Table V with Tables I and III). The resulting bubble shapes and curves for the benchmark quantities were in fact visually indistinguishable from the reference solution on all but the coarsest grids, and also significantly more accurate than those of the commercial codes.

The resulting errors together with reference values are shown in Table VI. From there it can be seen that Featflow TP2D produces very accurate results, and even on the very coarsest grid the error was significantly smaller than anything that the commercial codes could achieve.

IV. CONCLUSIONS

In this study two modern commercial simulation tools have been directly compared with a newly developed academic code to assess their capabilities to simulate two-phase flows with immersed interfaces. The chosen test problem was a rising bubble benchmark test case for which an accurate reference solution has been established. Computations were performed on different grid levels while measuring the required CPU time and simultaneously calculating the error in the circularity.

Fig. 5 shows the time averaged error against the CPU time for the different codes. It is clear that the solution produced by Comsol Multiphysics initially had quite a large error but also converged at a high rate due to the higher order Q_2P_1 finite element discretization. Unfortunately, solutions at very fine grids were practically impossible to compute due to the strong dependence on direct solvers. Ansys Fluent on the other hand started with a somewhat lower initial error but converged much slower. By the third grid level Fluent and Comsol had achieved roughly the same level of efficiency and surprisingly further refinements yielded no improvements at all, Fluent completely stopped converging. The academic TP2D code converged with first order and showed a much better overall efficiency, requiring about ten times less effort to achieve a certain accuracy than the commercial codes would have had they been able to compute on finer grids. Note that even the error on the very coarsest grid was already lower that anything that either of the commercial codes could produce.

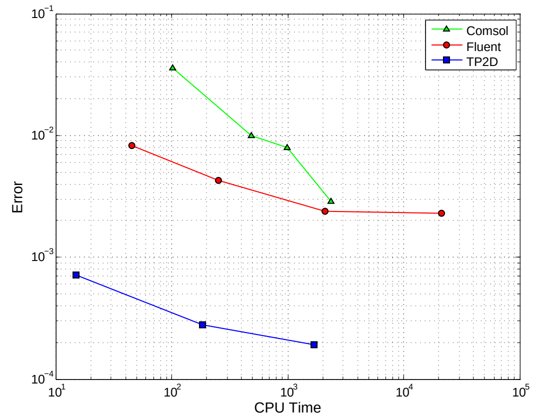

Fig. 5. Averaged error in the circularity vs. CPU time

Altogether, the newly developed FeatFlow TP2D simulation code has been rigorously validated together with two commercial codes by simulating a reference benchmark test case and comparing the resulting performance. The comparison highlighted real problems in the commercial codes and showed the merit of the academic approach which was able to outperform them by a magnitude or more.

V. ACKNOWLEDGMENTS

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