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A case-study in open-source CFD code verification, Part I: Convergence rate loss diagnosis

Original articles

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#### Abstract

This study analyzes the influence of cell geometry on the numerical accuracy of convection-diffusion operators in OpenFOAM. The large variety of solvers and boundary conditions in this tool, as well as the precision of the finite-volume method in terms of mesh quality, call for a verification process performed in steps. The work is divided into two parts. In the first (the current manuscript), we focus on the diffusion operator, which has been found to exhibit a loss in convergence rate. Although the cell-centered finite volume approach underlying OpenFOAM should preserve a theoretical second order convergence rate, loss of convergence order is observed when non-orthogonal meshes are used at the boundaries. To investigate the origins of this problem, the method of manufactured solutions is applied to yield analytical solutions for the Poisson equation and compute the numerical error. The root cause is identified and corrections to recover second-order convergence are proposed. In part two of this investigation, we show how convergence can be improved, and present results for problems described by the Poisson and Navier–Stokes equations.

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Keywords: Verification; Manufactured solution; OpenFOAM; CFD; Poisson equation

### 1. Introduction

Numerical calculations in fluid mechanics have developed considerably in recent decades, in part due to advances in computational power and in part because of advances in numerical methods. However, despite this progress, the simulation of real-world problems with complex geometries remains a major challenge. In fact, analytical solutions do not exist for these problems, and instead the equations representing a particular physical problem are solved via numerical simulation, which involves the use of approximations from various sources.

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The finite volume method (FVM), based on the laws of conservation, is currently one of the methods most often used to solve the Navier–Stokes equations for predicting industrial flows. Theoretical support for FVM on complex geometries can be found in the Computational Fluid Dynamics (CFD) literature [25,2], and [9].

OpenFOAM<sup>®</sup>, a trademark of The OpenFOAM Foundation, is a free, open source software package that is widely used for fluid flow simulations in both industry and academia. OpenFOAM's theoretical support, based on cell-centered finite volume discretization, includes a large variety of solvers, schemes, and processing tools for solving a wide range of problems in computational fluid mechanics. OpenFOAM support and theoretical background can be found in [11–13,15,16,14,17,18,20].

Flow simulations are routinely performed in industry, and OpenFOAM accuracy must be verified on the meshes that usually accompany the complex geometries in these simulations. Because of the complexity and extent of OpenFOAM libraries and tools, the verification process has to be performed in steps. However, there is little in the literature on the verification of OpenFOAM schemes, which is why we are addressing this important issue here. A background discussion, along with definitions and descriptions for some terms related to confidence building in CFD, was presented by Roache [23] and extended by Stern et al. [26]. There, validation is described as solving the right equations, and verification as solving the equations in the right way. The various aspects discussed in Roache's paper include the distinction between code verification and code validation, between the verification of code and the verification of calculations, grid convergence vs. iterative convergence, and numerical error vs. conceptual modeling error.

Along these lines, Abanto et al. [1] presented a grid convergence study on some atypical CFD cases using a number of commercial CFD packages. Their verification test cases are distinctive in that exact solutions are known. Verification test cases include the classical Poiseuille flow, an incompressible recirculating flow, a manufactured incompressible laminar boundary layer flow, and an incompressible annular flow. Different convergence rates are determined using structured and unstructured meshes. Stern et al. [26] describe a set of verification, validation, and certification methodologies and procedures for numerical simulations. Examples of the application of quantitative certification of Reynolds-Averaged Navier–Stokes (RANS) codes are presented for ship hydrodynamics.

In Tremblay et al. [27], the method of manufactured solutions (MMS) for fluid-structure interaction code verification is applied. These researchers observed that, when used with systematic grid refinement, MMS provides strong code verification. Roy et al. [24] used MMS to verify the order of accuracy of two finite-volume Euler and Navier–Stokes codes. These exact solutions were used to accurately evaluate the discretization error in the numerical solutions. Through global discretization error analysis, the spatial order of accuracy was observed to be second order for a node-centered approach using unstructured meshes. More recently, Iannelli [10] compared an exact solution and CFD solutions of the Navier–Stokes equations. They determined the convergence rates and orders of accuracy of these solutions and illustrated the utility of the exact solution developed for verification purposes. There is a series of published papers on MMS for 2D incompressible Navier–Stokes and turbulent models, which includes those by Eca and Hoekstra [6,7] and Eca et al. [8].

A recent study regarding verification for an unstructured finite volume CFD code has been published by Veluri and Roy [29], in which MMS is used to generate exact solutions to both the Euler and Navier-Stokes equations to verify the order of accuracy of the code on different grid types in 2D and 3D. The various options for code verification include the baseline steady-state governing equations, transport models, turbulence models, boundary conditions, and unsteady flows. Diskin et al. [5] studied the accuracy and complexity in finite volume discretization schemes for viscous fluxes on general grids using a node-centered scheme and three cell-centered schemes (a node-averaging scheme and two schemes using least-squares face-gradient reconstruction). Among several interesting results, they found that the node-averaging scheme has the highest complexity and can fail to converge to the exact solution when the node-averaged values are clipped. On highly anisotropic grids, the least-squares schemes, the node-averaging scheme without clipping, and the node-centered scheme demonstrated similar second-order accuracies per degree of freedom. Overall, the accuracies of the node-centered and the best cell-centered schemes are comparable at an equivalent number of degrees of freedom on isotropic and curved anisotropic grids. A similar work for inviscid fluxes is presented by Diskin and Thomas [3], the second-order cell-centered and node-centered approaches for finite volumes were compared for unstructured grid discretizations in two dimensions. Some weaknesses were observed in all these schemes, such as instability, accuracy degradation, and/or poor convergence of defect-correction iterations. In a more recent work, Diskin and Thomas [4] studied the effects of mesh regularity on the accuracy of unstructured node-centered finite-volume discretizations. In their paper, they focused on an edge-based approach which uses unweighted least-squares gradient reconstruction with a quadratic fit.

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