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Code verification for multiphase flows using the method of manufactured solutions[☆]

Aniruddha Choudhary[a,b,*], Christopher J. Roy[b], Jean-François Dietiker[c], Mehrdad Shahnam[a], Rahul Garg[a], Jordan Musser[a]

[a] National Energy Technology Laboratory, Morgantown, WV 26507, USA
[b] Aerospace and Ocean Engineering Department, Virginia Tech, Blacksburg, VA 24061, USA
[c] West Virginia University Research Corporation, Morgantown, WV 26506, USA

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ABSTRACT

Code verification is the process of ensuring, to the extent possible, that there are no algorithm deficiencies and coding mistakes (bugs) in a scientific computing simulation. Order of accuracy testing using the Method of Manufactured Solutions (MMS) is a rigorous technique that is employed here for code verification of the main components of an open-source, multiphase flow code – MFIX. Code verification is performed here on 2D and 3D, uniform and stretched meshes for incompressible, steady and unsteady, single-phase and two-phase flows using the two-fluid model of MFIX. Currently, the algebraic gas-solid exchange terms are neglected as these can be verified via techniques such as unit-testing. The no-slip wall, free-slip wall, and pressure outflow boundary conditions are verified. Temporal orders of accuracy for first-order and second-order time-marching schemes during unsteady simulations are also assessed. The presence of a modified SIMPLE-based algorithm in the code requires the velocity field to be divergence free in case of the single-phase incompressible model. Similarly, the volume fraction weighted velocity field must be divergence-free for the two-phase incompressible model. A newly-developed curl-based manufactured solution is used to generate manufactured solutions that satisfy the divergence-free constraint during the verification of the single-phase and two-phase incompressible governing equations. Manufactured solutions with constraints due to boundary conditions as well as due to divergence-free flow are derived in order to verify the boundary conditions.

Introduction

With increased use of computational tools for engineering simulations of complex physical systems, it becomes important to perform verification and validation studies for various aspects of a computational simulation. For a Computational Fluid Dynamics (CFD) simulation, verification and validation activities are useful in assessing the correctness of the code, quantifying the numerical accuracy of the simulation, and determining the applicability of the selected mathematical model. Verification deals with the mathematics of the simulation and involves assessing the correctness of the computer code and numerical algorithms as well as the accuracy of the numerical solution. Validation deals with the physics of the model and assesses whether the selected mathematical model satisfactorily predicts the physics of interest.

Verification in scientific computing can be categorized into code verification and solution verification. Code verification is the process of examining whether or not there are coding mistakes (bugs) in the computer code and inconsistencies in the algorithm. Solution verification is the process of identifying and estimating different forms of errors present in numerical simulations: discretization error, iterative convergence error, and round-off error. The different criteria for assessing code verification are: expert judgment, error quantification, consistency/convergence, and order of accuracy (Roy, 2005). Out of these, the order of accuracy test is the recommended acceptance test for rigorous code verification (Knupp and Salari, 2003; Roy, 2005; Oberkampf and Roy, 2010). Order of accuracy test requires the evaluation of discretization error on multiple grid levels. Discretization error is defined as the difference between the numerical solution to the discretized equations and the exact solution to the partial differential (or in-

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* Corresponding author at: Aerospace and Ocean Engineering Department, Virginia Tech, Blacksburg, VA 24061, USA. Tel.: +1 540 239 4824.
E-mail address: aniruddhac@gmail.com (A. Choudhary).

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tegral) equations. Evaluation of discretization error requires the knowledge of the exact solution for the governing equations which is certainly not known for problems of practical interest. In this scenario, a technique called the Method of Manufactured Solutions (MMS) (Roache and Steinberg, 1984) can be used where a solution is "manufactured" and used as an exact solution. This manufactured solution exactly solves the modified governing equations obtained by adding certain source terms (or forcing functions) to the original governing equations; the source terms are obtained by substituting the manufactured solution into the original governing equations. MMS is based upon the philosophy that code verification deals with the mathematics of the problem and hence arbitrary functions (with certain requirements as discussed later) can be selected as exact solutions. The books by Roache (2009), Knupp and Salari (2003), and Oberkampf and Roy (2010) provide a comprehensive discussion of code verification, MMS, and order of accuracy tests.

CFD simulations of fluid-solids multiphase systems can be categorized into two basic types: (1) continuum approaches, and (2) Lagrangian–Eulerian approaches. In a continuum approach, which is also referred to as the Eulerian–Eulerian method or the Two-Fluid Method (TFM), the different phases are mathematically described as interpenetrating continua and the governing equations for mass, momentum, and energy are obtained by averaging quantities over a control volume. The interaction between different phases is modeled using various sub-models commonly referred to as constitutive relations or closure models. The constitutive relations can be used to formulate interphase exchange terms describing various physical interactions such as momentum transfer and heat transfer between fluids and solid, or solid and solid phases (e.g., see Lun et al., 1984; Gidaspow, 1994; Oliveira and Issa, 1994 for discussion on modeling of interphase exchange terms). Special constitutive relations (such as interphase drag models, solid-stress models) are needed for practical problems of interest and are developed based upon experiments, or theoretical modeling, or first-principles based numerical simulations (such as direct numerical simulations, (e.g. Tenneti et al., 2011)). Although assessment and improvement of multiphase constitutive models are important processes in multiphase flow dynamics, they are not the main focus of the current work. Methods where the carrier (or surrounding) phase is treated as a continuum and the dispersed phase is treated as discrete entities (i.e., particles or parcels of particles) are called Lagrangian–Eulerian methods or continuum discrete methods. The code verification of Lagrangian–Eulerian methods is not directly addressed in the current study. However, the methodology presented here is useful for verification of a continuum discrete multiphase model if the carrier-phase equations employ an Eulerian framework.

Previous work

Code verification of multiphase flows is not as common in the literature as that for single-phase flows. This is due to the presence of approximately twice as many governing equations in multiphase flows compared to single-phase flows, complex interphase interaction terms, and several constitutive relations which make it difficult to obtain manufactured solutions or simple exact solutions for these equations. Grace and Taghipour (2004) discussed the importance of verification and validation activities for CFD models as applied to fluidized beds and other dense multiphase flow systems. In addition, they correctly concluded from a survey of articles claiming "verification" or "validation" for numerical models simulating fluidized beds that these terms have often been used inconsistently with their accepted terminology.

There have been some MMS-based multiphase code verification studies in a multi-material context. "Multiphase" in this sense refers to the presence of materials in the domain with different physical properties thus resulting in solution discontinuities at the material interface. Roache et al. (1990) used MMS to verify a finite-difference ground flow code with discontinuous conductivities in the domain by selecting the manufactured solutions such that they explicitly satisfy the geological boundary conditions. Crockett et al. (2011) applied MMS to verify a multi-material heat equation solver that uses a Cartesian cut-cell/embedded boundary method to represent the interface between the materials. In works by Roache et al. (1990) and Crockett et al. (2011), the interface locations are considered to be fixed and known a priori. Brady et al. (2012) presented a way to apply MMS to the finite volume multiphase code OSM which is a structured, Cartesian grid code for solving the heat equation. Manufactured solutions were generated using Heaviside and Dirac-delta functions to include the presence of moving interfaces in the domain for a typical immiscible two-phase system. They concluded that with such a discontinuity in material properties, the order of accuracy must reduce to first order for a second or higher order discretization scheme. This conclusion is also supported by Banks et al. (2008) who showed that the formally second order accuracy of the discrete system reduces to first order in the presence of nonlinear discontinuities and to non-integer values below one for linear discontinuities.

Shunn et al. (2012) used MMS to verify an unstructured variable density flow-solver for a miscible two-fluid system with manufactured solutions reflective of the physical behavior common to combustion problems such as convective propagation of density fronts and mixing of species through diffusion. Physically-realistic manufactured solutions for incompressible, single-phase flows were also proposed by Eça et al. (2007, 2012) for code verification of turbulent, wall-bounded flows. Vedovoto et al. (2011) performed a MMS-based code verification study of a pressure-based finite volume numerical scheme suited to variable density, single-phase flows generally encountered in combustion applications. In their work, the authors selected a manufactured solution mimicking the propagation of a corrugated flame front separating heavy from light gases. In all these studies, the manufactured solutions proposed satisfied the necessary criteria such as divergence-free velocity field, wall boundary conditions, or consistency with employed turbulence functions. There are some advantages in using such physically-realistic manufactured solutions in cases such as turbulence model verification (Eça et al., 2012) where the function and roles of different terms change based upon the nature of the solution. However, the selected manufactured solution should not just be realistic but also exhibit enough variations to ensure that all terms in the governing equations are exercised during the verification test (Pelletier and Roache, 2000; Pelletier, 2010).

Current work

The focus of current work is code verification of the discretized terms present in the two-fluid model governing equations. We use manufactured solutions that are mathematically general functions consisting of sinusoidal terms. This selection of manufactured solutions ensures a rigorous verification of all the discretized terms of the governing equations. The algorithm implemented in the code being investigated (i.e., MFIX, version 2014-1 (National Energy Technology Laboratory, 2014)) requires that the volume-fraction weighted velocity field be divergence-free for the selected manufactured solutions. We incorporate this constraint in the current work by introducing a novel, curl-based method to derive manufactured solution for code verification of incompressible flows. We also verify three of the most commonly used boundary conditions, i.e., no-slip wall, free-slip wall, and pressure outflow. While verifying these boundary conditions, we derive the manufactured solutions to satisfy the divergence-free velocity field constraint as