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Bubble tracking analysis of PWR two-phase flow simulations based on the level set method

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ABSTRACT

Bubbly flow is a common natural phenomenon and a challenging engineering problem yet to be fully understood. More insights from either experiments or numerical simulations are desired to better model and predict the bubbly flow behavior. Direct numerical simulation (DNS) has been gaining renewed interests as an attractive approach towards the accurate modeling of two-phase turbulent flows. Though DNS is computationally expensive, it can provide highly reliable data for model development along with experiments. The ever-growing computing power is also allowing us to study flows of increasingly high Reynolds numbers. However, the conventional simulation and analysis methods are becoming inadequate when dealing with such 'big data' generated from large-scale DNS. This paper presents our recent effort in developing the advanced analysis framework for two-phase bubbly flow DNS. It will show how one can take advantage of the 'big data' and translate it into in-depth insights. Specifically, a novel bubble tracking method has been developed, which can collect detailed two-phase flow information at the individual bubble level. Due to the importance of subcooled boiling phenomenon in pressurized water reactors (PWR), the bubbly flow is simulated within a PWR subchannel geometry with the bubble tracking capability. It has been demonstrated that bubble tracking method significantly improves the data extraction efficiency for level-set based interface tracking simulations. Statistical analysis was introduced to post-process the recorded data to study the dependencies of bubble behavior with local flow dynamics.

1. Introduction

Two-phase bubbly flow is quite common in various engineering applications, such as chemical industry (where presence of bubbles can increase the contact area for gas-liquid reactions), the oil production (where bubbles are injected to help lift thick heavy oil to surface), and energy generation plants (where boiling is the key process to generate the stream to drive turbines). As an example in nuclear engineering, the water in a PWR core serves as both the coolant and neutron moderator. By absorbing the heat from nuclear fuel rods, water coolant boils and generates steam bubbles. When appropriate amount of bubbles is generated in the PWR core, the heat removal efficiency from fuel rods can be significantly improved under proper safety margin (Kunugi, 2012). Therefore, a fundamental understanding of bubble behavior is important for both maintaining the operation stability and optimizing the efficiency. The nuclear community has seen the continuous research over decades to study the turbulent two-phase flow both experimentally (Trupp and Azad, 1975; Wheeler et al., 2015) and computationally (Lopez de Bertodano et al., 1994; Vaidheeswaran et al., 2017). In the meantime, as the Gen IV reactors being developed, more accurate and higher fidelity models are desired to further enhance the nuclear safety and efficiency. Given the extreme conditions and complex support structures in nuclear reactor cores, it is very challenging (if not impossible) to study the two-phase flow behavior with high-fidelity experiments. Instead, the validated computational approaches are commonly utilized as a practical means to predict two-phase flow behavior for thermal-hydraulics design and safety margin evaluation.

Thanks to the tremendous growth of computing power, there has been a renewed interest in applying DNS to study the nuclear engineering related flow problems (Ninokata et al., 2004; Fang et al., 2017). Equipped with a sufficiently fine mesh, DNS can resolve all turbulence structures down to Kolmogorov scales (Pope, 2000). DNS involves no turbulence models and can be coupled with interface tracking methods (ITM) to create a promising methodology to study two-phase turbulent flows. Recent DNS investigations on two-phase flows have revealed unprecedented insights into complex flow phenomena (Lu and Tryggvason, 2008; Bolotnov, 2013; Thomas et al., 2015). The development of new closure laws for multiphase

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computational fluid dynamics (M-CFD) and subchannel analysis can utilize the detailed information provided by the high-fidelity interface tracking simulations (ITS) of bubbly flows with the DNS of liquid turbulence.

As one of the major ITM, level set method (Sussman et al., 1994) is utilized in the presented research due to following three desirable features: (a) it can provide accurate representation of interfacial quantities, such as interface normal and curvature; (b) it makes no assumptions about the connectivity of the interface, which can allow topological transition (e.g. bubble coalescence or breakup) occur automatically without user intervention or extra coding; (c) it can be easily coupled with finite element method and unstructured mesh to provide simulations of two phase flow in very complicated geometries, such as a 2 × 2 PWR fuel rod bundle with spacer grid and mixing vanes (Fang and Bolotnov, 2014). The level set method makes use of a signed distance field, and the gas–liquid interface is modeled by the zero level-set. It can be readily used to distinguish phases based on the sign of the corresponding level-set value (e.g. the sign is positive in the liquid phase while negative in the gas phase). However, the traditional level-set is not able to collect calculated values and associate with specific bubbles when multiple bubbles present in the simulations. This drawback hinders the collection of valuable bubble information, which can give us in-depth insights about bubbly flow behavior. For example, how the different local fluid conditions could affect bubble interfacial forces, bubble deformation level, and eventually the bubble distribution throughout the entire domain. As a response to the need of new data analysis techniques, a novel bubble tracking methodology has been developed for level set ITM. Statistical analysis tools are also developed to process data extracted from bubble tracking simulations.

This article presents a comprehensive review of the newly developed bubble tracking method. In the demonstration study, a single PWR subchannel geometry is chosen as the computational domain. The liquid turbulence is fully resolved by DNS while the two-phase behaviors are captured by level set ITM. The hydraulics Reynolds number ($Re_h = \overline{U}D_h/\nu$) is 80,774 based on a hydraulic diameter ($D_h = 4A/P_w$) and mean velocity ($\overline{U}$). There are 262 bubbles (0.6509 mm in diameter each) initialized in the domain representing a 1% gas volume fraction. The simulated flow condition is roughly 1/5 of that under normal operating PWR environment in terms of Re_h (Fang et al., 2017). The current study is part of our effort approaching the realistic PWR conditions by considering the state-of-the-art computing resources. The application of bubble tracking capability is presented. The results obtained indicate a promising potential of the bubble tracking method.

2. Numerical method

The bubble tracking capability is developed within the PHASTA code, which is a three-dimensional finite element method (FEM) flow solver for both incompressible and compressible flows. Equipped with a level set algorithm, PHASTA is capable to simulate various two-phase flows (Nagrath et al., 2006; Bolotnov et al., 2011). In addition, PHASTA supports unstructured grid, which makes it feasible for simulations of turbulent flows in complex geometries, such as a 2 × 2 PWR structure with spacer grids and mixing vanes. Together with the highly scalable performance on massively parallel computers, PHASTA is a promising tool for advanced modeling of turbulent two-phase flows. The outstanding scalability of PHASTA has already been demonstrated (Rasquin et al., 2014), and the code has shown good scaling up to 768 × 1024 processors on the IBM Blue Gene/Q Mira system at Argonne National Laboratory (#9 fastest supercomputer in the world as of June 2017).

2.1. Governing equations

PHASTA solves the Incompressible Navier-Stokes (INS) equations directly in three dimensions using a stabilized finite element method (FEM) (Whiting and Jansen, 2001). The spatial and temporal discretization of INS equations within PHASTA has been discussed previously by Nagrath et al. (2005). The fluid is assumed to be isothermal in presented research. The strong form of INS is given by

$$\text{Continuity:} \frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\text{Momentum:} \rho\frac{\partial u_i}{\partial t} + \rho u_j\frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + f_i \tag{2}$$

where u_i is the velocity in the i-th dimension ($i = 1$, 2 and 3), ρ denotes the density of the fluid, p the static pressure and τ_{ij} the viscous stress tensor. f_i represents the i-th component of the body force vector. For the incompressible flow of a Newtonian fluid, the viscous stress tensor is related to the fluid viscosity μ and the strain rate tensor, S_{ij}, as:

$$\tau_{ij} = 2\mu S_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{3}$$

Employing the Continuum Surface Force (CSF) model proposed by Brackbill et al. (1992), the surface tension force is modeled as a local volumetric force density across the interface region (included in f_i).

2.2. Level set method

Introduced by Osher and Sethian (1988) and further developed by Sussman et al. (1994), the level-set method has been widely used as one of the major interface tracking approaches in multiphase flow simulations. PHASTA incorporates level-set method to extend the simulation capability from single-phase to two-phase flows (Nagrath et al., 2006). The bubble interface is modeled as the zero-level set of a smooth function, φ, where φ is called the first scalar and is represented as the signed distance from the zero-level set. That is, at $\varphi = 0$, the level set defines the interface. The scalar, φ, is advected with the fluid according to the advection Eq. (4) as described by Sussman et al. (1994).

$$\frac{\partial \varphi}{\partial t} + u_j\frac{\partial \varphi}{\partial x_j} = 0 \tag{4}$$

The liquid phase is indicated by a positive level set, $\varphi > 0$, while the gas phase by the negative, $\varphi < 0$.

Evaluating the jump in physical properties across gas-liquid interface using a step change is challenging numerically; therefore, the properties near the interface are determined using a smoothed Heaviside kernel function, H_ε (Bolotnov et al., 2011). While the solution may be relatively good in the close vicinity of the interface, the distance field, φ, may not be correct elsewhere in the domain where the varying fluid velocities would distort the level set contours (such as in a fully resolved turbulent flow). To maintain a true distance field, the level set field is corrected at every time iteration with a re-distancing operation, also known as re-initialization process (Fatemi and Sussman, 1995). A detailed description of the equations and re-distancing process was presented by Bolotnov et al. (2011).

2.3. DNS mesh design

The following requirements must be met to ensure an accurate representation of relevant turbulent scales in PHASTA simulations: (a) the computational domain must be sufficiently large to contain the largest turbulent eddies, and (b) the grid spacing must be sufficiently fine to capture the small scales of interest. The periodic inlet/outlet condition is adopted to allow properly resolving large turbulent eddies in the flow. To meet the second prerequisite, the mesh cell sizes should be comparable to the Kolmogorov length scale. For example, for the first layer of mesh cells upon the wall, the designed cell size is 3.25 μm while at the same location *a posteriori* Kolmogorov length scale is 2.85 μm. In the current study, the post-processing analysis suggests a range of