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Direct numerical simulation of reactor two-phase flows enabled by high-performance computing

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ABSTRACT

Nuclear reactor two-phase flows remain a great engineering challenge, where the high-resolution two-phase flow database which can inform practical model development is still sparse due to the extreme reactor operation conditions and measurement difficulties. Owing to the rapid growth of computing power, the direct numerical simulation (DNS) is enjoying a renewed interest in investigating the related flow problems. A combination between DNS and an interface tracking method can provide a unique opportunity to study two-phase flows based on first principles calculations. More importantly, state-of-the-art high-performance computing (HPC) facilities are helping unlock this great potential. This paper reviews the recent research progress of two-phase flow DNS related to reactor applications. The progress in large-scale bubbly flow DNS has been focused not only on the sheer size of those simulations in terms of resolved Reynolds number, but also on the associated advanced modeling and analysis techniques. Specifically, the current areas of active research include modeling of sub-cooled boiling, bubble coalescence, as well as the advanced post-processing toolkit for bubbly flow simulations in reactor geometries. A novel bubble tracking method has been developed to track the evolution of bubbles in two-phase bubbly flow. Also, spectral analysis of DNS database in different geometries has been performed to investigate the modulation of the energy spectrum slope due to bubble-induced turbulence. In addition, the single- and two-phase analysis results are presented for turbulent flows within the pressurized water reactor (PWR) core geometries. The related simulations are possible to carry out only with the world leading HPC platforms. These simulations are allowing more complex turbulence model development and validation for use in 3D multiphase computational fluid dynamics (M-CFD) codes.

1. Introduction

In engineering applications, which usually involve complex geometries and high Reynolds number flows, a full-scale DNS calculation may not be a practical solution yet. However, the continuous growth of computing power has led to a strong interest in applying DNS to various flow problems (Kim et al., 1987; Ninokata et al., 2004; Fang et al., 2017). Although the computational cost remains the major bottleneck in the near future, DNS approach is valued as a reliable data source along with experiments. The optimism about DNS is supported by several favorable evidences:

- DNS could provide high-fidelity and fundamental insights to complex fluid phenomena, such as the turbulence anisotropy (Bolotnov, 2013);
- this approach allows to carefully study the separate effects of various parameters (Thomas et al., 2015);
- the tremendous growth of high performance computing (HPC) is making expensive simulations more and more affordable (Rasquin et al., 2014).

In DNS of turbulence, the equations of fluid motion (i.e. the Navier-Stokes equations) are solved without any turbulence closure assumptions; unlike other CFD techniques such as eddy viscosity modeling or LES where modeling assumptions are essential to the problem. Given sufficient temporal and spatial resolution, DNS can represent all the scales of turbulence down to the Kolmogorov scales (Kolmogorov, 1942). Thanks to its predictive capability based on first principles calculations, DNS is widely accepted as a reliable data source for model development and validation (Pope, 2000). In addition, compared to

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experiments, numerical simulations provide more degrees of control regarding the flow conditions (Prosperetti and Tryggvason, 2007). It allows researchers to perform comprehensive parametric studies for the parameters of interest. Furthermore, some challenging flow environments are more feasibly represented in numerical simulations than experiments, such as the turbulent coolant flow inside nuclear reactor cores at high temperature/pressure conditions, reducing the ecological and economic impact required to perform similar experiments (when those are possible to implement).

Coupled with interface tracking methods, the DNS capability can be extended from the single-phase turbulent flow to two-phase. This extension usually relies on a marker (i.e. phase indicator) function that can be advected by the flow. The phase indicator function plays two important roles: (1) it is used to determine interface location and represent interface topology change; (2) it is used to determine the material properties of different phases, such as density and viscosity. There are three mainstream interface tracking methods: volume of fluid method (Hirt and Nichols, 1981), front tracking method (Unverdi and Tryggvason, 1992) and level set method (Sussman et al., 1994). The solution techniques of these three approaches are all based on the "one-fluid" formulation. The one-fluid formulation allows multiphase flow with interfaces to be treated as a single fluid that has different properties on each side of the interface. Using this approach, the Navier-Stokes equations for both phases can be solved in a single system of equations using variable material properties determined by the phase indicator function.

The specific interface tracking method used in the present research is the level set method, which was first introduced by Osher and Sethian (1988) and further developed by Sussman et al. (1994). The level set method utilizes a signed distance field to represent the phases separated by an interface, and the interface is modeled by zero level set. The level set calculations consist of an advection step and a re-distancing/re-initialization step. Since the initial introduction of level set method into multiphase simulations, it has been widely used as one of the major interface tracking methods. Level set method is selected herein due to the following three desirable features: (a) level set method can provide accurate representation of interfacial quantities, such as interfacial normal vector and surface curvature; (b) level set method makes no assumptions about the connectivity of the interface, which can allow topological transition (e.g. bubble coalescence or breakup) to occur automatically without user intervention or extra coding; (c) level set method can be easily coupled with finite element method and unstructured mesh to provide simulations of two-phase flow in very complicated geometries, such as 2 × 2 PWR structure with spacer grid and mixing vanes (Yi et al., 2014).

The past forty years have seen increasingly rapid advances in the field of HPC. Because of this favorable trend, the scale of high-fidelity numerical simulations has significantly expanded. A brief history of selected single- and two-phase DNS studies is illustrated in Fig. 1. As pioneers, Moser and his collaborators have applied DNS in turbulence studies of fully developed single-phase channel flow (Moser and Moin, 1984, Kim et al., 1987, Moser et al., 1999, Lee and Moser, 2015). The hydraulic Reynolds number (Re_h) resolved in their work has evolved progressively from 11,960 to the latest 500,000 considering the channel hydraulic diameter as the characteristic length scale. It is worthwhile to mention that the Re_h of 500,000 is already higher than that one could expect under realistic PWR coolant flow conditions (Fang et al., 2017). Researchers have become interested in applying DNS to nuclear related flow problems since the beginning of 21st century. For example, Ninokata et al. (2004) have employed DNS to analyze the fully developed single-phase turbulent flow in triangular fuel pin bundles, but the investigated Reynolds number is relatively low (up to 23,763).

As for the two-phase flow DNS, most research efforts in the past have been focused on simulating buoyant bubbles in simple periodic box domains (Unverdi and Tryggvason, 1992, Esmaeeli and Tryggvason, 1998, Tryggvason et al., 2001). The designated Reynolds number is generally defined based on bubble-induced velocity and bubble size (i.e. bubble diameter). The simulation scale therein usually ranges from 10^3 to 10^5 in terms of grid points. However, in recent years, the scale of two-phase flow DNS in terms of mesh resolution and resolvable flows has grown significantly and is likely to keep growing (Bolotnov et al., 2011, Bolotnov, 2013, Tryggvason and Lu, 2015, Fang et al., 2017). In Fig. 1, the converted hydraulic Reynolds number Re_h is referred for all cited DNS studies. While the single-phase DNS has already reached the realistic PWR flow conditions, the two-phase flow DNS in reactor geometries is expected to arrive at the same milestone in early 2020's given the access to next-generation HPC (e.g. the Aurora HPC being developed at Argonne National Laboratory (ANL)). The main reason for being behind is twofold: (i) interface tracking simulations are more expensive due to additional equations being solved and more strict meshing requirements to resolve the interface curvature; (ii) nuclear reactor core geometries require unstructured meshes which involve different discretization methodologies inherently more expensive than Cartesian geometry approaches.

For the DNS study with increasingly high Re_h, the corresponding mesh discretization would result in large amount of mesh elements/regions. This also allows representing a considerable number of bubbles in the domain. One of the latest two-phase DNS conducted at North Carolina State University (NCSU) successfully advected over 3000 bubbles in a vertical pipe domain. Even more bubbles would be expected in the future DNS investigations. The analysis of the turbulence as well as the bubble behavior will become a serious challenge at that scale. In the meantime, to accurately represent all important physics involved in reactor two-phase flows, advanced two-phase models are also demanded, such as the modeling of boiling phenomenon. In summary, DNS capability has just recently started to overlap with problems

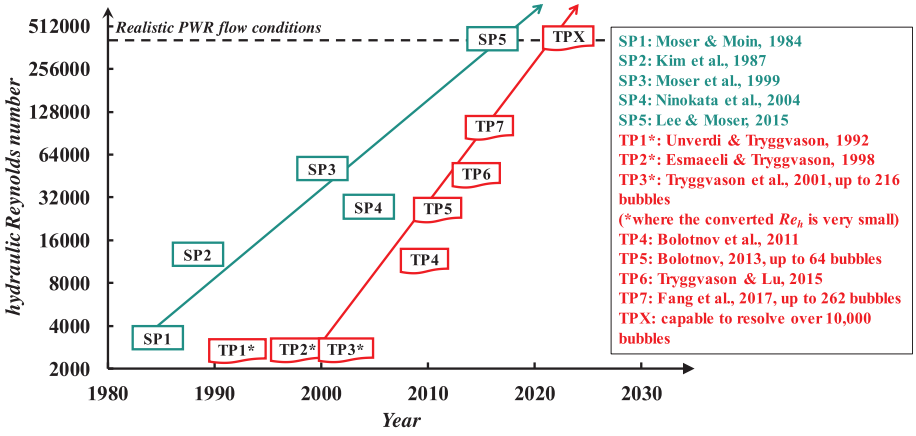

Fig. 1. The scale of single-phase (SP) and two-phase (TP) DNS studies in terms of investigated hydraulic Reynolds number and its evolution over time.