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Applications of high-resolution spatial discretization scheme and Jacobian-free Newton–Krylov method in two-phase flow problems

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ABSTRACT

The majority of the existing reactor system analysis codes were developed using low-order numerical schemes in both space and time. In many nuclear thermal–hydraulics applications, it is desirable to use higher-order numerical schemes to reduce numerical errors. High-resolution spatial discretization schemes provide high order spatial accuracy in smooth regions and capture sharp spatial discontinuity without nonphysical spatial oscillations. In this work, we adapted an existing high-resolution spatial discretization scheme on staggered grids in two-phase flow applications. Fully implicit time integration schemes were also implemented to reduce numerical errors from operator-splitting types of time integration schemes. The resulting nonlinear system has been successfully solved using the Jacobian-free Newton–Krylov (JFNK) method. The high-resolution spatial discretization and high-order fully implicit time integration numerical schemes were tested and numerically verified for several two-phase test problems, including a two-phase advection problem, a two-phase advection with phase appearance/disappearance problem, and the water faucet problem. Numerical results clearly demonstrated the advantages of using such high-resolution spatial and high-order temporal numerical schemes to significantly reduce numerical diffusion and therefore improve accuracy. Our study also demonstrated that the JFNK method is stable and robust in solving two-phase flow problems, even when phase appearance/disappearance exists.

1. Introduction

The majority of the existing reactor system analysis codes, such as RELAP5 (RELAP5, 2001) and TRAC (TRAC, 2001), were originally developed in the mid- to late 1970s. They have played very important roles in the nuclear engineering field by supporting reactor safety analyses as well as design and licensing of new reactors. These codes employed low (first) order numerical methods in both space and time to solve the one-dimensional, two-phase flow equations in reactor systems. The disadvantages of using low-order numerical methods have long been realized in the nuclear thermal–hydraulics field. The classic Implicit Continuous-Fluid Eulerian (Harlow and Amsden, 1968, 1971) type of operator-splitting method (also known as the semi-implicit method) is commonly used as the time integration scheme. The method introduces a first-order numerical error in time from the operator-splitting process, and it is subject to the material Courant–Friedrichs–Lewy (CFL) stability limit. For spatial discretization, staggered grid mesh combined with the donor cell upwind method is generally used in existing codes for its simplicity, stableness, and ability to preserve monotonicity. However, these schemes are highly diffusive and not always desirable in many applications such as boron solute transport. As new reactor designs emerge, there are new challenges appearing in numerical simulations of reactor systems, such as long transient problems and strongly coupled multi-physics problems. As we aim to improve the numerical accuracy of reactor safety analysis codes, it is important to consider advanced numerical schemes and methods. Our approach includes three aspects. These include: (1) high-resolution spatial discretization scheme in order to improve the spatial accuracy; (2) fully implicit time integration schemes in order to allow large time step and to improve the temporal accuracy; and (3) advanced solving method (such as the Jacobian-free Newton–Krylov (JFNK) method) to efficiently solve the highly nonlinear system.

High-resolution spatial discretization schemes are able to maintain higher-order accuracy in smooth regions while nonphysical spatial oscillations are removed or significantly reduced near discontinuities. However, there have been very few attempts to apply such high-resolution methods in the nuclear thermal–hydraulics

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field. In addition, most of these works use explicit time integration schemes (Tiselj and Petelin, 1997; Munkejord, 2006; Macián-Juan, 1996; Bertolotto et al., 2011), or semi-implicit schemes already implemented in existing system analysis codes (RELAP5-3D, 2012; Wang, 2012; Wang et al., 2013). For example, Tiselj and Petelin (1997) made an attempt to apply a high-resolution scheme to solve the two fluid, two-phase flow equations. Special treatments have been done to render the equation system to be hyperbolic in order to use their second-order accurate scheme based on a high-resolution shock capturing method. The explicit time integration method was used. Some of the other existing works are limited to apply high-resolution spatial schemes on scalar variables only, such as boron solute (Macián-Juan, 1996; Bertolotto et al., 2011; RELAP5-3D, 2012), or mass/energy equations only (Wang, 2012; Wang et al., 2013). A second-order accurate Godunov method was implemented in RELAP5-3D to solve the boron transport equation (RELAP5-3D, 2012). However, that scheme is limited to solve the boron transport equation only, and it is lack of thorough tests in system applications according to reference RELAP5-3D (2012). Macián-Juan (1996) did an early work to improve the spatial accuracy of boron transport in the system analysis code TRAC using the QUICKEST-ULTIMATE type of flux limiter scheme for one-dimensional flows. Bertolotto et al. (2011) has also implemented the same method in the TRACE code to improve the spatial accuracy of the dissolved solute convection equation. This method was developed to use an explicit time integration scheme, and it was applied to the solute equation only. Recently, Wang (2012), Wang and his coworkers (Wang et al., 2013) reported their works on the implementation and assessment of a high-resolution numerical method in TRACE. The high-resolution scheme was applied for the mass and energy equations only, and no treatment was done for the momentum equation. A more restrictive condition on the time-step size than the default CFL limit was also reported in Wang's work (Wang, 2012).

Fully implicit methods are not commonly seen in reactor safety analysis codes, with CATHARE (Bestion, 1990; Barre et al., 1992) as one of the rare exceptions. Attempts to apply Newton's method in solving fully implicit two-phase flow problems can be found in Frepoli's work (Frepoli et al., 2003) and Abu Saleem's work (Abu Saleem and Kozlowski, 2014). High-resolution spatial scheme was also used in Abu Saleem's work (Abu Saleem and Kozlowski, 2014), and promising results were obtained. In recent years, the Jacobian-free Newton–Krylov method (Knoll and Keyes, 2004) has gained increasing interest for solving large nonlinear systems. In two-phase flow simulations, Mousseau did several pioneering works (Mousseau, 2004, 2005, 2006) to use such a method to solve two-phase flow problems implicitly. All Mousseau's works, however, were focused on a first-order upwind spatial discretization scheme. A recent work to apply the JFNK method in solving two-phase flow problems was done by Ashrafizadeh et al. (2015). The spatial discretization scheme is based on a cell centered AUSM+ method, however they were not able to correctly simulate the phase appearance/disappearance problem using the JFNK method.

In this work, it is our objective to investigate the high-resolution spatial discretization scheme on the staggered grid mesh, as well as high-order fully implicit time integration schemes, in the applications of two-phase flow problems. The resulting nonlinear system will be solved by the JFNK method. These numerical schemes could potentially form a foundation to solve the two-phase flow problems with better numerical accuracy. In Section 2, the problem descriptions are given for the simplified two-phase flow problems. In Section 3, the high-resolution scheme on staggered grid we adapted in this work, along with the time integration schemes and the JFNK method will be briefly discussed. In Section 4, the applications of high-resolution spatial discretization and high-order implicit time integration schemes on several two-phase flow test problems will be presented. Discussions and conclusions are presented in Section 5.

2. Problem descriptions

For the two-phase flow model, we are particularly interested in the two-fluid, single pressure, two-phase flow equations, which are commonly used in the existing system analysis codes such as RELAP5 (RELAP5, 2001), TRAC (TRAC, 2001), and CATHARE (Bestion, 1990). Since the main purpose is to demonstrate the advantages of using advanced numerical schemes, a simplified version of the two-fluid, single pressure, two-phase flow equations are used in this work. Focusing on the two-phase flow hydrodynamics, and ignoring the mass transfer between the two phases, and wall and interfacial frictions, the six-equation system is further reduced to a four-equation system, including two mass equations and two momentum equations:

$$\frac{\partial(\alpha_l\rho_l)}{\partial t} + \frac{\partial[\alpha_l\rho_l u_l]}{\partial x} = 0 \tag{1}$$

$$\frac{\partial(\alpha_g\rho_g)}{\partial t} + \frac{\partial(\alpha_g\rho_g u_g)}{\partial x} = 0 \tag{2}$$

$$\frac{\partial u_l}{\partial t} + u_l\frac{\partial u_l}{\partial x} + \frac{1}{\rho_l}\frac{\partial p}{\partial x} - g = 0 \tag{3}$$

$$\frac{\partial u_g}{\partial t} + u_g\frac{\partial u_g}{\partial x} + \frac{1}{\rho_g}\frac{\partial p}{\partial x} - g = 0 \tag{4}$$

in which the subscripts l and g denote the liquid phase and the gas phase, respectively. The variables to be solved from this set of equations are p, α_g, u_l, and u_g, which are pressure, void fraction (volume fraction of the gas phase), liquid phase velocity, and gas phase velocity, respectively. Note that $\alpha_l = 1 - \alpha_g$. To close the equation system, linearized equations of state were used for both phases:

$$\rho_l(p) = 1000 + 10^{-7}(p - 10^5); \quad \rho_g(p) = 0.5 + 10^{-6}(p - 10^5) \tag{5}$$

3. Numerical and solution methods

In this section, we will briefly discuss: (1) a high-resolution spatial discretization scheme based on staggered grid mesh arrangement, (2) fully implicit time integration schemes, and (3) the JFNK method in solving the nonlinear equation system.

3.1. High-resolution staggered grid spatial discretization

In this work, we adapted a high-resolution spatial discretization scheme on staggered grid mesh, which can be found in the original work done by Stelling and Duinmeijer (2003). The reason that we choose the staggered grid mesh is because it is flexible to handle the two-phase equations in primitive forms, and it is compatible with most existing system analysis codes. The high-resolution scheme was obtained by introducing the linear reconstruction of the variable solutions and slope limiter into the original first-order upwind method. For the purpose of completeness, the spatial discretization scheme is briefly discussed in this subsection.

For the staggered grid mesh commonly used in existing reactor safety system codes, scalar variables (such as pressure and density) are arranged in cell centers, while vector variables (such as velocity) are arranged on cell edges.

$$\left.\frac{\partial(\alpha_g\rho_g u_g)}{\partial x}\right|_i = \frac{1}{\Delta x}\left[(\alpha_g\rho_g u_g)^*_{i+1/2} - (\alpha_g\rho_g u_g)^*_{i-1/2}\right] \tag{6}$$

and