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# Application of continuous adjoint method to steady-state two-phase flow simulations

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ABSTRACT

Verification, validation and uncertainty quantification (VVUQ) have become a common practice in thermal-hydraulics analysis. An important step in the uncertainty analysis is the sensitivity analysis of various uncertainty input parameters. The common approach for computing the sensitivities, e.g. variance-based and regression-based methods, requires solving the governing equation multiple times, which is expensive in terms of computational effort. An alternative approach for computing the sensitivities is the adjoint method. The cost of solving an adjoint equation is comparable to the cost of solving the governing equation. Once the adjoint solution is obtained, the sensitivities of various parameters can be obtained with little effort. However, successful adjoint sensitivity analysis of the two-phase flow is rare. In this work, an adjoint sensitivity analysis framework is developed for the two-phase two-fluid model based on a new upwind numerical solver. The adjoint sensitivity analysis framework is tested with a steady-state boiling pipe problem. Results show that the adjoint sensitivity analysis framework is working as expected. The sensitivities obtained with the adjoint method are verified by the sensitivities obtained with a forward method.



## 1. Introduction

In recent years, verification, validation and uncertainty quantification (VVUQ) have become a common practice in thermal-hydraulics analysis. In general, these activities deal with propagation of uncertainties in computer code simulations, e.g. through system analysis codes. An important step in uncertainty analysis is the sensitivity analysis of various uncertain input parameters. A common approach to calculate sensitivity includes variance-based and regression-based methods. However, these methods require solving the system of interest (in our case, two-phase flow) multiple times, sometimes 100s of times, using different input parameters, which is very expensive in terms of CPU time. An alternative approach for calculating sensitivities is the adjoint method. The cost of solving an adjoint equation is comparable to the cost of solving the governing equation (forward equation, e.g. the two-phase two-fluid model equation). However, once the adjoint solution is obtained, the sensitivity to an arbitrary number of parameters can be calculated at the same time.

There is a long history of using the adjoint method in optimal control theory. The use of adjoint method for computing sensitivities came up in the nuclear industry in the 1940s. Later, the adjoint method became popular in computational fluid dynamics field (Marchuk, 1995; Giles and Pierce, 2000). Within the field of aeronautical computational fluid dynamics, the use of adjoint method has been seen in (Jameson, 1988, 1994; Jameson et al., 1998; Nadarajah and Jameson, 2000). Adjoint problems arise naturally in the formulation of methods for optimal aerodynamic design and optimal error control (Giles et al., 1998, 2000, 2001; Giles et al., 2003). Adjoint solution provides the linear sensitivities of an objective function (e.g. lift force and drag force) to a number of design variables. These sensitivities can then be used to drive an optimization procedure. In a sequence of papers, Jameson developed the adjoint approach for the potential flow, the Euler equation, and the Navier-Stokes equation (Jameson, 1988, 1994; Jameson et al., 1998; Nadarajah and Jameson, 2000). Many of these methods were based on the continuous form of the governing equation. These methods belong to the group of so-called continuous adjoint method (Marchuk, 1995).

The application of the adjoint method to optimal aerodynamic design is very successful. However, to the author's best knowledge, successful adjoint sensitivity analysis of the two-phase flow problems is rare. Cacuci performed an adjoint sensitivity analysis to two-phase flow problems using the RELAP5 MOD3.2 numerical discretization (Cacuci and Wacholder, 1982; Cacuci and Ionescu-Bujor, 2000a,b). This method belongs to a group of so-called discrete adjoint method (Marchuk, 1995). An application of Cacuci's

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approach was illustrated by Petruzzi, 2008, where the approach was applied to the blowdown of a gas from a pressurized vessel.

The objective of this paper is to develop an adjoint sensitivity analysis framework for two-phase flow problems using the continuous adjoint method. At first, a forward solver is built based on an approximate Riemann solver to solve the two-phase flow problems. Then, an adjoint sensitivity analysis framework is developed based on the forward solver. Finally, a numerical test with the Christensen boiling pipe problem is performed to verify the adjoint sensitivity analysis framework.

## 2. Forward solver

### 2.1. Flow model

For 1D problems, the basic two-phase two-fluid six-equation model without any differential closure laws (Ishii and Hibiki, 2010; Team, 2012a; Bajorek et al., 2008) can be written in a compact vector form as

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F}}{\partial x}+\mathbf{P}_{ix}\frac{\partial \alpha_g}{\partial x}+\mathbf{P}_{it}\frac{\partial \alpha_g}{\partial t}=\mathbf{S} \tag{1}$$

where $\mathbf{U}$ is the vector of conservative variables, $\mathbf{F}$ is the vector of flux variables, $\mathbf{P}_{ix}$ and $\mathbf{P}_{it}$ are the vectors related to the partial derivatives of the void fraction, and $\mathbf{S}$ is the vector of source terms. They are defined as

$$\begin{aligned}
\mathbf{U}&\equiv\begin{pmatrix}\alpha_l\rho_l\\ \alpha_l\rho_l u_l\\ \alpha_l\rho_l E_l\\ \alpha_g\rho_g\\ \alpha_g\rho_g u_g\\ \alpha_g\rho_g E_g\end{pmatrix},\quad \mathbf{F}\equiv\begin{pmatrix}\alpha_l\rho_l u_l\\ \alpha_l\rho_l u_l^2+\alpha_l p\\ \alpha_l\rho_l H_l u_l\\ \alpha_g\rho_g u_g\\ \alpha_g\rho_g u_g^2+\alpha_g p\\ \alpha_g\rho_g H_g u_g\end{pmatrix}\\
\mathbf{W}&\equiv\begin{pmatrix}\alpha_g\\ p\\ T_l\\ T_g\\ u_l\\ u_g\end{pmatrix},\quad \mathbf{P}_{ix}\equiv\begin{pmatrix}0\\ p\\ 0\\ 0\\ -p\\ 0\end{pmatrix},\quad \mathbf{P}_{it}\equiv\begin{pmatrix}0\\ 0\\ -p\\ 0\\ 0\\ p\end{pmatrix}
\end{aligned} \tag{2}$$

This model assumes all pressure terms, including phasic pressure and interfacial averaged pressure, are equal. Let the subscript $k=l,g$ denote the liquid phase and gas phase, respectively. The variables $(\alpha_k,\rho_k,u_k,e_k)$ denote the volume fraction, the density, the velocity, and the specific internal energy of $k$-phase. The summation of phasic volume fraction should be one, i.e. $\alpha_l+\alpha_g=1$. $p$ is the pressure of two phases. $E_k=e_k+u_k^2/2$ and $H_k=e_k+p/\rho_k+u_k^2/2$ are the phasic specific total energy and specific total enthalpy. Note that one more vector, $\mathbf{W}$, is introduced to denote the physical variables. The source vector $\mathbf{S}$ is modeled as

$$\mathbf{S}=\begin{pmatrix}-\Gamma_g\\ -\alpha_l\rho_l g-f_{wl}+f_i-\Gamma_g u_i\\ Q_{wl}+Q_{il}-\Gamma_w h_l'-\Gamma_{ig}h_l^*+(f_i-f_{wl}-\alpha_l\rho_l g-\Gamma_g u_i)u_l+\Gamma_g\frac{u_l^2}{2}\\ \Gamma_g\\ -\alpha_g\rho_g g-f_{wg}-f_i+\Gamma_g u_i\\ Q_{wg}+Q_{ig}+\Gamma_w h_g'+\Gamma_{ig}h_g^*+\left(-f_i-f_{wg}-\alpha_g\rho_g g+\Gamma_g u_i\right)u_g-\Gamma_g\frac{u_g^2}{2}\end{pmatrix} \tag{3}$$

where $\Gamma_g$ is the net vapor generation rate due to wall vapor generation ($\Gamma_w$) and bulk vapor generation ($\Gamma_{ig}$), $u_i$ is the interface velocity, $f_i$ is the interfacial friction, $f_{wk}$ is the phasic wall friction, $Q_{ik}$ is the phasic interfacial heat flux, $Q_{wk}$ is the phasic wall heat flux, $h_k'$ is the phasic enthalpy carried by the wall vapor generation term ($\Gamma_w$), and $h_k^*$ is the phasic enthalpy carried by the bulk vapor generation term ($\Gamma_{ig}$). Correlations based on RELAP5-3D code manual (Team, 2012a; Team, 2012c) are used to model these variables.

An appropriate Equation of State (EOS) is required to close the system. For many practical problems in the nuclear thermal–hydraulics analysis, the temperature of two phases are required to model the source terms. In such a case, a useful EOS is given by specifying the Gibbs free energy as a function of pressure and temperature $T_k$, i.e.

$$\mathfrak{g}_k=\mathfrak{g}_k(T_k,p),\quad \text{for } k=l,g \tag{4}$$

After specifying the specific Gibbs free energy, the phasic density and specific internal energy are obtained from the partial derivatives of the specific Gibbs free energy. The details about specifying the EOS through the specific Gibbs free energy are referred to (Wagner and Kruse, 1998; Hu, 2018).

### 2.2. Numerical method

For 1D problems, the spatial discretization is shown schematically in Fig. 1. For simplicity of the notation, a uniform spatial discretization is considered. All unknown variables are stored in the cell center (co-located mesh). On each side of the physical domain, ghosts cells are used to deal with the boundary conditions.

The system is updated in time with the forward Euler method, i.e.

$$\mathbf{U}_i^{n+1}=\mathbf{U}_i^n+\Delta t\mathcal{L}^\dagger(\mathbf{U}_i^n) \tag{5}$$

where the time step is determined by the Courant-Friedrichs and Lewy (CFL) condition

$$\Delta t=\mathrm{CFL}\frac{\Delta x}{\lambda_{\max}} \tag{6}$$

where $\lambda_{\max}$ is the maximum wave speed (eigenvalue) at the current time step.

$\mathcal{L}^\dagger$ contains the discretization of the differential terms and the source terms, i.e.

$$\mathcal{L}^\dagger(\mathbf{U}_i^n)=-\frac{\hat{\mathbf{F}}_{i+\frac{1}{2}}-\hat{\mathbf{F}}_{i-\frac{1}{2}}}{\Delta x}-\mathbf{P}_{ix,i}^n\frac{\alpha_{g,i+1}^n-\alpha_{g,i-1}^n}{2\Delta x}-\mathbf{P}_{it,i}^n\frac{\left(\alpha_{g,i}^n-\alpha_{g,i}^{n-1}\right)}{\Delta t}+\mathbf{S}_i^n \tag{7}$$

where $\hat{\mathbf{F}}_{i+1/2}$ and $\hat{\mathbf{F}}_{i-1/2}$ are numerical fluxes at cell boundaries. The $\mathbf{P}_{it}\partial\alpha_g/\partial t$ part is approximated with a first-order finite difference method and $\mathbf{P}_{ix}\partial\alpha_g/\partial x$ is approximated with second-order central-difference method. In this paper, a Roe-type numerical flux $\hat{\mathbf{F}}_{i+1/2}^{\mathrm{Roe}}$ (Toro, 2013; Glaister, 1988) is used.

Let $\mathbb{A}_c$ be a 6-by-6 matrix defined as

$$\mathbb{A}_c\equiv\frac{\partial \mathbf{F}}{\partial \mathbf{U}} \tag{8}$$

Let $\lambda_{c,m}$ and $\mathbf{K}_{c,m}$, for $m=1,\ldots,6$ be the eigenvalues and right eigenvectors of the matrix $\mathbb{A}_c$. The subscript $c$ denotes that the Jacobian matrix and eigenvalues/eigenvectors are obtained with the

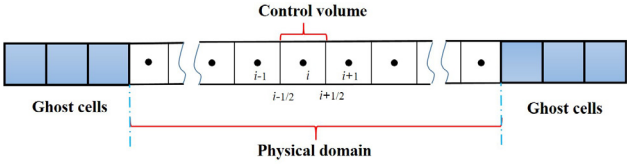


**Fig. 1.** Schematic of the 1D spatial discretization.