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Application of Adjoint Sensitivity Analysis Procedure to Single Phase Thermal-Hydraulics with Heat Structure Code

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1. Introduction

In the thermal hydraulic analysis domain of nuclear system, mass, momentum and energy conservation equations for multiple phases are often solved with a set of selected empirical constitutive equations to close the problem. The heat structure equations are also coupled with conservations equations, to obtain the safety analysis results of the heat structure and the coolant. The analysis procedure needs numerous variables and parameters as an input. To optimize the safety analysis procedure for nodes, options and so on, sensitivities of each variables and parameters need to be calculated. Local Adjoint Sensitivity Analysis Procedure(ASAP) is developed by Cacuci[1,2,3] to calculate the system responses locally around a chosen point in the combined phase-space of parameters and space variables. The method has the advantage of less required computational resources. In this study, the authors are going to apply the ASAP to 1-D single-phase transient analysis code with heat structure.

2. Review of ASAP of Single-Phase Thermal Hydraulics Code and Extension of ASAP to Heat Structure

In this section, the authors firstly reviewed the past derivation of adjoint sensitivity analysis procedure to single phase thermal-hydraulic system code[4].

2.1 Governing equation of single phase thermal-hydraulic code and heat equation

A separate single-phase transient analysis code, named to NTS code, is consisted of following three equations. Eq. 1 is mass continuity equation, Eq. 2 and 3 represent the momentum conservation equation and energy conservation equation respectively. The code solves three equations for three variables, such as pressure, temperature and velocity.

$$\frac{\partial}{\partial t}(\rho_l) + \frac{1}{A}\frac{\partial}{\partial x}(\rho_l v_l A) = 0 \tag{1}$$

$$\rho_l A\frac{\partial v_l}{\partial t} + \frac{1}{2}\rho_l A\frac{\partial v_l^2}{\partial x} = -A\frac{\partial P}{\partial x} + \rho_l B_x A - (\rho_l A)\mathrm{FWF}(v_l) \tag{2}$$

$$\frac{\partial}{\partial t}(\rho_l U_l) + \frac{1}{A}\frac{\partial}{\partial x}(\rho_l U_l v_l A) = -\frac{P}{A}\frac{\partial}{\partial x}(v_l A) + Q_{wl} + DISS_l \tag{3}$$

These equations are expressed with the Eqs 4-7. X is a vector which represents dependent variables, and G is a vector which represents parameters.

$$N(\mathbf{X},\boldsymbol{G}) - S(\boldsymbol{G}) = 0 \tag{4}$$

$$\mathbf{X} = (P,T,v) \tag{5}$$

$$\mathbf{X}(x,t_0) = \mathbf{X}_{init}(x) \tag{6}$$

$$\mathbf{X}(x_0,t) = \mathbf{X}_{bound}(t) \tag{7}$$

In the past study, ASAP application to single-phase system thermal-hydraulic analysis code, only the adjoint sensitivity analysis was done for the conservation equations. To calculate response, which is calculated by NTS code[5], following eq 8, 9,10 is used.

$$R(\mathbf{X},\boldsymbol{G}) \equiv \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx F[\mathbf{X}(x,t),\boldsymbol{G}(x,t)] \tag{8}$$

$$N(\mathbf{X}^0 + \mathbf{\Phi}, \boldsymbol{G}^0 + \mathbf{\Gamma}) - S(\boldsymbol{G}^0 + \mathbf{\Gamma}) = 0 \tag{9}$$

$$\mathbf{\Phi} \equiv (\Phi_1,\Phi_2,\Phi_3) = (\delta P, \delta T, \delta v) \tag{10}$$

To calculate the sensitivity of a response to parameter variation, Gateaux- (G-) differential is used. By the G-differential, the sensitivity DR is expressed with Eq. 11. To calculate sensitivity with eq. 11, eq. 12 should be solved firstly. This method is called as forward sensitivity analysis procedure.

$$DR(\mathbf{X}^0,\boldsymbol{G}^0;\mathbf{\Phi},\mathbf{\Gamma}) \equiv \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left\{\int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx F[\mathbf{X}^0+\epsilon\mathbf{\Phi}, \boldsymbol{G}^0+\epsilon\mathbf{\Gamma}]\right\}_{\epsilon=0} = \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx \left(\frac{\partial F}{\partial \boldsymbol{G}}\right)^0 \mathbf{\Gamma}(x,t) + \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx \left(\frac{\partial F}{\partial \mathbf{X}}\right)^0 \mathbf{\Phi}(x,t) \tag{11}$$

$$\sum_{n=1}^{3}\left\{\frac{\partial}{\partial t}[S_{mn}(x,t)\Phi_n(x,t)] + \frac{1}{A^0(x)}\times\frac{\partial}{\partial x}[A^0(x)T_{mn}(x,t)\Phi_n(x,t)] + U_{mn}(x,t)\Phi(x,t)\right\} \equiv \boldsymbol{L\Phi} = \sum_{j=1}^{J} Q_{mj}(x,t)\Gamma_j(x,t) \tag{12}$$

To decrease computational cost, ASAP[2] is introduced to calculate the sensitivity DR. By defining $\mathbf{\Phi}^*$ as Eq.13 and take inner product with Eq.12, Eq.14 can be used by definition of adjoint operator[2].

$$\mathbf{\Phi}^*(x,t) \equiv (\Phi_1^*(x,t),\Phi_2^*(x,t),\Phi_3^*(x,t)) \tag{13}$$

$$\langle \mathbf{\Phi}^*, \boldsymbol{L\Phi}\rangle = \langle \boldsymbol{M}\mathbf{\Phi}^*, \mathbf{\Phi}\rangle + \{P[\mathbf{\Phi},\mathbf{\Phi}^*]\} \tag{14}$$

To obtain adjoint sensitivity analysis equations for NTS code, following operations [3] are performed to Eq. 14.

1. Set $\mathbf{M\Phi}^* = \left(\frac{\partial \mathrm{F}}{\partial \mathbf{X}}\right)^0$
2. To eliminate unknown value $\mathbf{\Phi}(\mathrm{x},\mathrm{t_f})$ and $\mathbf{\Phi}(\mathrm{x_f},\mathrm{t})$, set $\mathbf{\Phi}^*(\mathrm{x},\mathrm{t_f}) = 0$ and $\mathbf{\Phi}^*(\mathrm{x_f},\mathrm{t}) = 0$

Then, following Eq. 15 is obtained, and the vector adjoint function $\mathbf{\Phi}^*$ satisfies adjoint equations, represented as Eq. 16. With Eq. 11 and Eq. 15, the sensitivity DR is expressed as Eq. 17.

$$\langle\left(\frac{\partial \mathrm{F}}{\partial \mathbf{X}}\right)^{0}, \boldsymbol{\Phi}\rangle = \langle \boldsymbol{\Phi}^{*}, \boldsymbol{L\Phi}\rangle + \int_{x_0}^{x_f} \boldsymbol{\Phi}^{*}(x,t_0)[\boldsymbol{S}(x,t_0)\cdot \Delta\mathbf{X}(x,t_0)]dx + \int_{t_0}^{t_f} \boldsymbol{\Phi}^{*}(x_0,t)[\boldsymbol{T}(x_0,t)\cdot \Delta\mathbf{X}(x_0,t)]dt \quad (15)$$

$$\sum_{n=1}^{3}\left\{-S_{nm}\frac{\partial \Phi_n^*}{\partial t} - A^0 T_{nm}\frac{\partial \Phi_n^*/A^0}{\partial x} + U_{nm}(x,t)\Phi_n^*(x,t)\right\} \equiv \left(\frac{\partial \mathrm{F}}{\partial \mathrm{X_m}}\right)^{0}, \text{ m=1, 2, 3} \quad (16)$$

$$DR(\mathbf{X}^0, \boldsymbol{G}^0; \boldsymbol{\Phi}, \boldsymbol{\Gamma}; \boldsymbol{\Phi}^*) = \sum_{j=1}^{J}\int_{x_0}^{x_f} dx \int_{t_0}^{t_f} dt \left(\frac{\partial F}{\partial g_j}\right)^0 \gamma_j + \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx \boldsymbol{\Phi}^* \cdot (\boldsymbol{Q\Gamma}) + \int_{x_0}^{x_f} \boldsymbol{\Phi}^*(x,t_0)[\boldsymbol{S}(x,t_0)\cdot \Delta\mathbf{X}(x,t_0)]dx + \int_{t_0}^{t_f} \boldsymbol{\Phi}^*(x_0,t)[\boldsymbol{T}(x_0,t)\cdot\Delta\mathbf{X}(x_0,t)]dt \quad (17)$$

The system of adjoint equations, Eq. 16, shows the important characteristics of adjoint sensitivity analysis. The adjoint function is independent of parameter variation, since it does not include parameter variation terms. Thus the adjoint function is independent of parameter variation. Next, the source term of adjoint equation relies on the response R. Thus, Eq.16 needs to be solved for every R. From these characteristics, computational cost of adjoint sensitivity analysis is much cheaper when the number of parameter variations is larger than the number of response.

2.2 Extension of ASAP to with heat equation

In the nuclear system industry, the system analysis code used for the safety analysis of the nuclear system, not only the governing equation of the fluid but also the heat conduction equation of the heat structure are solved together to show the analysis result. Eq. 18 shows the heat conduction equation in structure (cylindrical fuel rod), which is applied in this study.

$$\rho_h C_{ph}\frac{\partial T_h}{\partial t} - \frac{1}{r}\frac{\partial}{\partial r}\left(rk_h\frac{\partial T_h}{\partial r}\right) - S = 0 \quad (18)$$

For the heat conduction equation, Eq. 19 and 20 is used as boundary condition in original code system.

$$\frac{\partial T_h}{\partial r} = 0, r = 0 \quad (19)$$

$$k_h\frac{\partial T_h}{\partial r} + h[T_h - T_\mathrm{f}] = 0, r = R \quad (20)$$

To calculate response of the system code, which is coupled with heat conduction equation, eq. 21 is used.

$$R(\mathrm{T}_h, P, U, v; \alpha) = \int_{x_i}^{x_o} dx \int_0^R rdr \int_{t_i}^{t_o} F(\mathrm{T}_h, P, U, v; \alpha)dt \quad (21)$$

With the G-differential to eq. 21, the sensitivity of the coupled system is calculated, in eq 22.

$$\delta R\left(\mathrm{T}_h^0, P^0, U^0, v^0; \alpha^0; \delta\mathrm{T}_h, \delta P, \delta U, \delta v; \delta\alpha\right) = \frac{d}{d\epsilon}\left\{\int_{x_i}^{x_o} dx \int_0^R rdr \int_{t_i}^{t_o} F\left(\mathrm{T_h^0} + \epsilon\delta\mathrm{T}_h, P^0 + \epsilon\delta P, U^0 + \epsilon\delta U, v^0 + \epsilon\delta v; \alpha^0 + \epsilon\delta\alpha\right)dt\right\}_{\epsilon=0} = \delta R_{direct} + \delta R_{indirect} \quad (22)$$

The "direct effect" term can be computed directly from the parameter variation, however the "indirect effect" term cannot be calculated immediately, like the eq.11 and eq.12. The forward sensitivity analysis procedure should be done to calculate the sensitivity in eq. 22.

Simillarly, to decrease computational cost, the adjoint sensitivity analysis procedure is done for the coupled system, eq 1-3 and 18.

By the same method as for deriving the adjoint equation and adjoint sensitivity analysis procedure of the single phase thermal hydraulics code, the adjoint equation and adjoint boundary condition are derived.

$$A_{11}(T_h^*) + A_{12}(P^*) + A_{13}(U^*) + A_{14}(v^*) = \frac{\partial F}{\partial T_h} \quad (23)$$

$$A_{21}(T_h^*) + A_{22}(P^*) + A_{23}(U^*) + A_{24}(v^*) = \frac{\partial F}{\partial P} \quad (24)$$

$$A_{31}(T_h^*) + A_{32}(P^*) + A_{33}(U^*) + A_{34}(v^*) = \frac{\partial F}{\partial U} \quad (25)$$

$$A_{41}(T_h^*) + A_{42}(P^*) + A_{43}(U^*) + A_{44}(v^*) = \frac{\partial F}{\partial v} \quad (26)$$

Eq 23-26 are the adjoint equation to compute the adjoint function of the system code dependent variables. All of the components in the eq 23-26 is derived but not be presented in this paper, since the components are length and complicated. Eq 27-35 are the initial and boundary conditions be satisfied by the adjoint function.

$$T_h^*(t,r,x) = 0, t = t_f \quad (27)$$

$$\frac{\partial T_h^*(t,r,x)}{\partial r} = 0, at\ r = 0 \quad (28)$$

$$h(P,U,v,\alpha)T_h^*(t,r,x) + k_h(T_h^0;\alpha^0)\frac{\partial T_h^*(t,r,x)}{\partial r} = 0, at\ r = R \quad (29)$$

$$P^*(t,r,x) = 0, \mathrm{t} = \mathrm{t_f} \quad (30)$$

$$P^*(t,r,x) = 0, \mathrm{x} = \mathrm{x_{out}} \quad (31)$$

$$U^*(t,r,x) = 0, \mathrm{t} = \mathrm{t_f} \quad (32)$$

$$U^*(t,r,x) = 0, \mathrm{x} = \mathrm{x_{out}} \quad (33)$$

$$v^*(t,r,x) = 0, \mathrm{t} = \mathrm{t_f} \quad (34)$$

$$v^*(t,r,x) = 0, \mathrm{x} = \mathrm{x_{out}} \quad (35)$$

These equations and boundary conditions can be used to calculate the adjoint function to reduce the amount of computation required for the sensitivity dR. This process is called as adjoint sensitivity analysis procedure.

2.3 Preliminary result of Application of ASAP to Single Phase Thermal-Hydraulics with Heat Structure Code

Sensitivity calculations area performed using a simple model to verify the adjoint sensitivity analysis procedure using the sensitivity calculated using the adjoint equation and adjoint function derived above. The authors wrote an in-house code for the ASAP to single phase thermal-hydraulics with heat structure code. Figure 1 shows the simple pipe – heat structure coupled model.

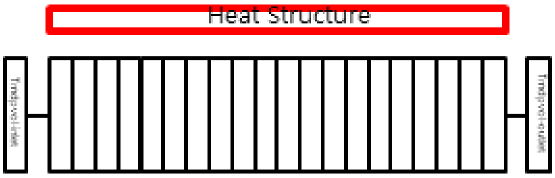

Figure 1. Single-pipe, single heat structure test model

For the test, the authors compute the pressure response sensitivities to the variation in the initial fluid velocity. By setting all parameter variations to zero, except for the variation δv_i, eq 36 shows the sensitivity.

$$\frac{\partial R}{\partial v_i(x;\alpha)}\delta \mathrm{v}_i(x;\alpha) = \int_{x_i}^{x_o} dx \int_0^R r dr\, U^*(t_i, r, x)\delta v_i(x;\alpha) \qquad (36)$$

Initial pressure of the pipe is 1.9255 * 10^5 Pa, initial velocity of the flow is 1.166m/s, and initial temperature of the fluid is 354.6K. Under these conditions, the current in-house code results are compared with sensitivity results which is calculated by repeating the original problem. From the in-house code of adjoint sensitivity analysis procedure model, the sensitivity value is 5.2638e4. However, from the repeating calculation, the sensitivity value is 1.4366e4. The sensitivity values are different, it is checked that the sensitivities of different types of comparison calculation are different from each other, but the tendency is the same.

3. Summary and Further Works

The authors reviewed adjoint sensitivity analysis procedure(ASAP) in this paper. The forward sensitivity analysis module and adjoint sensitivity analysis module for single-phase with heat structure code, which consists of three governing equations for single-phase flow, were derived. Implementation and preliminary verification of the adjoint sensitivity analysis module was done in this paper. In the case of the implementation of the adjoint sensitivity analysis procedure model, there are many points to check in the temporal discritization, spatial discritization and matrix calculation. The authors will perform verification and validation on these issues, and the result will be presented in the conference.

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