Application of Adjoint Sensitivity Analysis Procedure(ASAP) to Single Phase Thermal-Hydraulic System Analysis Code

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1. Introduction

In the nuclear system thermal hydraulic analysis domain, 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 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[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.

2. Methods

In this section, the authors will present governing equations of 1-D single-phase thermal hydraulic system analysis code, which is built in MATLAB environment by W. W. Lee and J. I. Lee[1] in section 2.1. The derivations of application of the ASAP[2] to the differential governing equation are presented in section 2.2. This is followed by implementing the ASAP[2] for discretized governing equation are presented in section 2.3

2.1 Governing equation

A separate single-phase transient analysis code, named to NTS code, is consisted of following three equations. Eq. 1 is mass continuity equation, Eqs. 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.

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

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

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

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

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

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

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

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

2.2 Adjoint Sensitivity Analysis Procedure for differential GEs

Response, which is calculated by NTS code, can be represented in the integral form of Eq. 8.

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

Response which is calculated with nominal parameters is expressed as $R^0(\mathbf{X}^0, \boldsymbol{G}^0)$, and the nominal parameter values have uncertainties(variations). The parameter variations are represented as $\boldsymbol{\Gamma} \equiv (\gamma_1, \gamma_2, \ldots, \gamma_J) = (\delta g_1, \delta g_2, \ldots, \delta g_J)$. When the parameter variations are applied to Eq. 4, the perturbed solution satisfies Eq. 9, $\boldsymbol{\Phi}$ is defined in Eq. 10.

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

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

To calculate the sensitivty of a response to parameter variation, Gateaux- (G-) differential is commonly used. Eq. 11 shows the definition of the G-differntial of an operator $F(\boldsymbol{e})$ at $\boldsymbol{e}^0$ with perturbation $\boldsymbol{h}$.

$$DF(\boldsymbol{e}^0, \boldsymbol{h}) \equiv \lim_{\epsilon \to 0} \epsilon^{-1}[F(\boldsymbol{e}^0 + \epsilon\boldsymbol{h}) - F(\boldsymbol{e}^0)] = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\{F(\boldsymbol{e}^0 + \epsilon\boldsymbol{h}\}_{\epsilon=0} \quad (11)$$

Now, sensitivity DR of the response is represented by Eq. 12. From Eq. 12, the sensitivity can be calculated after the function $\boldsymbol{\Phi}$ is determined. To determine $\boldsymbol{\Phi}$, G-differential is applied to differential GEs. Eq. 13 shows the G-differentials of differential GEs. To calculate the sensitivity DR, solution of Eq. 13 is used. This method is called as forward sensitivity analysis. Eq.13 needs to be solved for every γ_i, therefore its computational cost is expensive as the recalculations of Eqs. 4-7 and recalculations of perturbed response are necessary [3].

$$DR(\mathbf{X}^0, \boldsymbol{G}^0; \boldsymbol{\Phi}, \boldsymbol{\Gamma}) \equiv \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left\{\int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx F[\mathbf{X}^0 + \epsilon\boldsymbol{\Phi}, \boldsymbol{G}^0 + \epsilon\boldsymbol{\Gamma}]\right\}_{\epsilon=0} = \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx \left(\frac{\partial F}{\partial \boldsymbol{G}}\right)^0 \boldsymbol{\Gamma}(x,t) + \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx \left(\frac{\partial F}{\partial \mathbf{X}}\right)^0 \boldsymbol{\Phi}(x,t) \quad (12)$$

$$\sum_{n=1}^{3}\left\{\frac{\partial}{\partial t}[S_{mn}(x,t)\Phi_n(x,t)] + \frac{1}{A^0(x)} \times \frac{\partial}{\partial x}[A^0(x)T_{mn}(x,t)\Phi_n(x,t)] + U_{mn}(x,t)\Phi(x,t)\right\} \equiv \boldsymbol{L\Phi} = \sum_{j=1}^{J} Q_{mj}(x,t)\Gamma_j(x,t) \quad (13)$$

Therefore, to decrease computational cost, ASAP[2] is introduced to calculate the sensitivity DR. By defining $\mathbf{\Phi}^*$ as Eq.14 and take inner product with Eq.13, Eq.15 can be used by definition of adjoint operator[2].

$$\mathbf{\Phi}^*(x,t) \equiv (\Phi_1^*(x,t), \Phi_2^*(x,t), \Phi_3^*(x,t)) \quad (14)$$
$$\langle \mathbf{\Phi}^*, \boldsymbol{L}\mathbf{\Phi} \rangle = \langle \boldsymbol{M}\mathbf{\Phi}^*, \mathbf{\Phi} \rangle + \{P[\mathbf{\Phi}, \mathbf{\Phi}^*]\} \quad (15)$$

To obtain adjoint sensitivity analysis equations for NTS code, following operations [3] are performed to Eq. 15.

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. 16 is obtained, and the vector adjoint function $\mathbf{\Phi}^*$ satisfies adjoint equations, represented as Eq. 17. With Eq. 12 and Eq. 16, the sensitivity DR is expressed as Eq. 18.

$$\langle \left(\frac{\partial \mathrm{F}}{\partial \mathbf{X}}\right)^0, \mathbf{\Phi} \rangle = \langle \mathbf{\Phi}^*, \boldsymbol{L}\mathbf{\Phi} \rangle + \int_{x_0}^{x_f} \mathbf{\Phi}^*(x,t_0)[\boldsymbol{S}(x,t_0) \cdot \Delta\mathbf{X}(x,t_0)]dx + \int_{t_0}^{t_f} \mathbf{\Phi}^*(x_0,t)[\boldsymbol{T}(x_0,t) \cdot \Delta\mathbf{X}(x_0,t)]dt \quad (16)$$

$$\sum_{n=1}^{3} \left\{ -S_{nm} \frac{\partial \Phi_n^*}{\partial t} - A^0 T_{nm} \frac{\partial \Phi_n^*/A^0}{\partial x} + U_{nm}(x,t)\Phi_n^*(x,t) \right\} \equiv \left(\frac{\partial \mathrm{F}}{\partial \mathrm{X_m}}\right)^0, \text{ m=1, 2, 3} \quad (17)$$

$$DR(\mathbf{X}^0, \boldsymbol{G}^0; \mathbf{\Phi}, \mathbf{\Gamma}; \mathbf{\Phi}^*) = \sum_{j=1}^{J} \int_{x_0}^{x_f} dx \int_{t_0}^{t_f} dt \left(\frac{\partial F}{\partial g_j}\right)^0 \gamma_j + \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx \mathbf{\Phi}^* \cdot (\boldsymbol{Q}\mathbf{\Gamma}) + \int_{x_0}^{x_f} \mathbf{\Phi}^*(x,t_0)[\boldsymbol{S}(x,t_0) \cdot \Delta\mathbf{X}(x,t_0)]dx + \int_{t_0}^{t_f} \mathbf{\Phi}^*(x_0,t)[\boldsymbol{T}(x_0,t) \cdot \Delta\mathbf{X}(x_0,t)]dt \quad (18)$$

The system of adjoint equations, Eq. 17, shows the important characteristics of adjoint sensitivity analysis. First, it does not include parameter variation terms. Therefore, the adjoint function is independent of parameter variation. Second, the source term of adjoint equation relies on the response R. Thus, Eq.17 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.

2.3 Adjoint Sensitivity Analysis Procedure for discretized GEs

Actual code is consisted of discretized form of governing equations. Similarly, the response represented by Eq. 8 should be discretized to calculate numerically. Eqs. 19 and 20 denote discretized response and discretized sensitivity respectively[3].

$$R(\mathbf{X_d}, \boldsymbol{G}) = \sum_{n=0}^{NF} \sum_{j=1}^{NJ} \sum_{k=1}^{NV} F_{jk}^n(\mathbf{X}_d, \boldsymbol{G}) \quad (19)$$

$$DR = \sum_{n=0}^{NF} \sum_{j=1}^{NJ} \sum_{k=1}^{NV} \left[\sum_{v=1}^{3} \frac{\partial F_{jk}^n}{\partial \mathrm{X}_{d,v}} \Psi_v + \sum_{\alpha=1}^{J} \frac{\partial F_{jk}^n}{\partial g_\alpha} \gamma_\alpha \right] \equiv DR(\mathbf{\Psi}) + DR(\mathbf{\Gamma}) \quad (20)$$

To derive forward sensitivity analysis module for discretized GEs, following notations should be introduced.

1. Over a volume number k = 1,…,NV, at time step n, n = 1,…,NF, following notations are used for volume-averaged dependent variables.
$$(\mathbf{X}_k^1)^n = (\delta \mathrm{P})_k^n; (\mathbf{X}_k^2)^n = (\delta \mathrm{T})_k^n;$$
2. Over a junction number j = 1,…,NJ, at time step n, n = 1,…,NF, following notations are used for junction dependent variable
$$(\mathbf{Y}_j)^n = (\delta \mathrm{v})_j^n$$

Applying G-differential to Eq. 4, following matrices represent the discrete forward sensitivity analysis

$$\sum_{\nu=1}^{2} \left[\boldsymbol{BV}_{\mu\nu}^{n-1} \boldsymbol{X}_\nu^n + \boldsymbol{CV}_{\mu\nu}^{n-1} \boldsymbol{X}_\nu^{n-1} \right] + \boldsymbol{DV}_\mu^{n-1} \boldsymbol{Y}^n + \boldsymbol{EV}_\mu^{n-1} \boldsymbol{Y}^{n-1} = \boldsymbol{FV}_\mu^{n-1} \quad (21)$$
$$\mu = 1,2,3; \mathrm{n} = 1, \dots, \mathrm{NF}$$

$$\sum_{\nu=1}^{2} [\boldsymbol{BJ}_\nu^{n-1} \boldsymbol{X}_\nu^n + \boldsymbol{CJ}_\nu^{n-1} \boldsymbol{X}_\nu^{n-1}] + \boldsymbol{DJ}^{n-1} \boldsymbol{Y}^n + \boldsymbol{EJ}^{n-1} \boldsymbol{Y}^{n-1} = \boldsymbol{FJ}_\mu^{n-1} \quad (22)$$
$$\mathrm{n} = 1, \dots, \mathrm{NF}$$

$$\boldsymbol{BV}_{\mu\nu}^n = \left[(\mathrm{bv})_{\mathrm{ij}}^{\mu\nu}\right]_{(NV\times NV)}; \boldsymbol{CV}_{\mu\nu}^n = \left[(\mathrm{cv})_{\mathrm{ij}}^{\mu\nu}\right]_{(NV\times NV)}$$
$$\boldsymbol{DV}_\mu^n = \left[(\mathrm{dv})_{\mathrm{ij}}^{\mu\nu}\right]_{(NV\times NV)}; \boldsymbol{EV}_\mu^n = \left[(\mathrm{ev})_{\mathrm{ij}}^{\mu}\right]_{(NV\times NV)}$$
$$\boldsymbol{BJ}_\nu^n = \left[(\mathrm{bj})_{\mathrm{ij}}^{\mu\nu}\right]_{(NJ\times NV)}; \boldsymbol{CJ}_\nu^n = \left[(\mathrm{cj})_{\mathrm{ij}}^{\mu\nu}\right]_{(NJ\times NV)}$$
$$\boldsymbol{DJ}^n = \left[(\mathrm{dj})_{\mathrm{ij}}^{\mu\nu}\right]_{(NJ\times NV)}; \boldsymbol{EJ}^n = \left[(ev)_{ij}\right]_{(NJ\times NV)} \quad (23)$$

Eqs. 21 and Eq. 22 denote discretized GEs for volume and junction respectively. Vectors on the right side of Eq. 22 and Eq. 23 denote the parameter variation dependent terms. These equations are re-arranged in Eq. 25, by using the block matrix notations in Eq. 24.

$$\begin{bmatrix} \mathrm{BV}_{1,1} & \mathrm{BV}_{1,2} & DV_{1,1} \\ \mathrm{BV}_{2,1} & \mathrm{BV}_{2,2} & DV_{2,1} \\ BJ_{1,1} & BJ_{1,2} & DJ_{1,1} \end{bmatrix}_{3\times 3}^{(n)} \equiv \boldsymbol{B}^{(n)}$$
$$\begin{bmatrix} \mathrm{CV}_{1,1} & \mathrm{CV}_{1,2} & EV_{1,1} \\ \mathrm{CV}_{2,1} & \mathrm{CV}_{2,2} & EV_{2,1} \\ CJ_{1,1} & CJ_{1,2} & EJ_{1,1} \end{bmatrix}_{3\times 3}^{(n)} \equiv \boldsymbol{C}^{(n)} \quad (24)$$

$$\boldsymbol{B}^{(n-1)} \boldsymbol{X}^{(n)} + \boldsymbol{C}^{(n-1)} \boldsymbol{X}^{(n-1)} = \boldsymbol{F}^{(n-1)}$$
$$\boldsymbol{X}^{(0)} = \boldsymbol{F}^{init} \quad (25)$$

To apply the adjoint sensitivity analysis module to discretized GEs, a matrix equation Eq. 26 is multiplied to left side of Eq. 25, and the result is Eq. 27.

$$\Xi \equiv (\Xi^{(0)}, \dots, \Xi^{(NF)} \quad (26)$$
$\Xi^{(0)}$ is same size and structure as $\mathrm{X}^{(\mathrm{n})}$

$$\Xi^{\mathrm{T}} A \mathrm{X} = \sum_{n=0}^{NF} \Xi^{(n)} A^{(n)} \mathrm{X}^{(n)} \quad (27)$$

A represents a matrix composed of $B^{(n)}$ and $C^{(n)}$

Then, $DR(\mathbf{\Psi})$ can be expressed in the form of Eq. 28. Q is a source term in Eq. 19. Identifying Q with Eq. 29, adjoint sensitivity analysis module is given by Eq. 30.

$$DR(\mathbf{\Psi}) \equiv \mathrm{X}^{\mathrm{T}} A^{T} \Xi = \mathrm{X}^{\mathrm{T}} Q = \sum_{n=0}^{NF} \mathrm{X}^{(n)} Q^{(n)} = \Xi^{\mathrm{T}} A \mathrm{X} = \Xi^{\mathrm{T}} F = \sum_{n=0}^{NF} \Xi^{(n)} F^{(n)} \quad (28)$$

$$\mathrm{X}^{\mathrm{T}} A^{T} \Xi = \mathrm{X}^{\mathrm{T}} Q = \sum_{n=0}^{NF} \mathrm{X}^{(n)} Q^{(n)} \quad (29)$$

$$\left[B^{(NF-1)}\right]^{\mathrm{T}} \Xi^{(NF)} = Q^{(NF)}, \text{ for n} = \text{NF}$$
$$\left[B^{(n-1)}\right]^{\mathrm{T}} \Xi^{(n)} + \left[C^{(n-1)}\right]^{\mathrm{T}} \Xi^{(n)} = Q^{(n)} \text{ , for n} = \text{NF} - 1, \dots, 1$$
$$\Xi^{(0)} + \left[C^{(0)}\right]^{\mathrm{T}} \Xi^{(1)} = Q^{(0)}, \text{ for n} = 0 \quad (30)$$

By combining Eq. 19 and Eq. 28, the sensitivity DR of the response R is given in terms of adjoint function Ξ in Eq. 31.

$$DR \equiv DR(\mathbf{\Gamma}) + DR(\mathbf{\Psi}) = DR(\mathbf{\Gamma}) + \sum_{n=0}^{NF} \Xi^{(n)} F^{(n)} \quad (31)$$

The discrete adjoint sensitivity analysis module, Eq. 30, should be solved backward in time, from the final time step NF.

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 NTS code, which consists of three governing equations for single-phase flow, were derived. Implementation and verification of the adjoint sensitivity analysis module will be presented in the conference.

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