TOWARDS IMPLEMENTING DIRECT SENSITIVITY AND UNCERTAINTY METHODS IN THERMALHYDRAULIC CODES

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Abstract

Proper sensitivity and uncertainty analysis of thermalhydraulic codes is important due to the move from deterministic towards probabilistic strategies. Sensitivity analysis is generally performed using statistical methods for a limited number of important parameters treating the code as a black box simulation. Another option is a direct analytical approach through the use of partial derivatives. Analytical methods, though complex to employ, must only be done once and provide a wealth of sensitivity information that is relevant to any scenario modeled by the simulation. A possible process for applying direct analytical sensitivity analysis to a complex thermalhydraulics code is described herein.

1. Introduction

Uncertainty and sensitivity analysis are at the forefront of Nuclear Engineering research. The movement away from deterministic approaches has driven the need for methods which incorporate proper uncertainty quantification and analysis of uncertainty propagation through models and systems. Best estimate methods and probabilistic analysis, which seek to accurately define the state of a system with a given confidence level are emerging as replacements to the conservative approaches previously utilized in nuclear safety analysis. These methods require a thorough investigation of the uncertainties involved in a specific system or simulation to provide relevant conclusions. The effects of input uncertainties on simulation outputs is studied using sensitivity analysis methods to determine the effects of certain perturbed parameters on simulation results. A proper evaluation of the sensitivities provides information on the inner workings of the system that can be utilized to understand the propagation of input uncertainties through the code. Thus using input parameters with a quantified uncertainty and a robust sensitivity analysis of the system the output uncertainty of a simulation can be computed.

2. Direct Sensitivity and Uncertainty Analysis Methods

Code uncertainty and sensitivity to inputs are a connected process which seeks to determine how an uncertainty in input parameters will propagate through the simulation and the variations in output parameters that will be produced. By performing proper sensitivity analysis the uncertainty of the code output can be determined given a defined uncertainty in the inputs. In addition, the parameters that affect the output can be assed and ranked to determine the most important inputs. Sensitivity analysis can be performed using sampling methodologies or using direct analytical methods to determine the relationships between input and output parameters.

2.1 Sampling Methods for Sensitivity Analysis

Sensitivity analysis of a simulation can be performed by perturbing the inputs about their normal values to determine the effects on outputs of the system. Sampling methods will generate random values of an input parameter within a certain range and using a Monte Carlo method can produce a probabilistic output distribution for the given input distribution. It is through this assessment that a predicted response for the code can be generated with an acceptable confidence level. For each input parameter investigated an extensive amount of direct full code simulation is required to produce a robust representation of the output distribution. Once the output response is defined for the perturbation of a certain input the sensitivity of the output of that parameter can be numerically determined. The computational horsepower required for this assessment is quite high to generate a suitable distribution. In addition many cases must be run to determine the interaction between the input parameters that can be varied. Each perturbed input parameter may have a covariance with other input parameters requiring several combinations of perturbed parameters to be run. Also, the sensitivity of outputs may be different for various values of the input parameters. For certain analysis cases where the possible range of the inputs is high it is necessary to run multiple sets of cases to fully capture the input curve.

The computing demands may be reduced by taking a set of representative input combinations and performing a hundred to a thousand code runs in order to produce a Functional Response Surface (FRS). The FRS is usually a multivariable polynomial curve fit of the code response which can approximate the real modelling code with sufficient accuracy. The FRS is then run instead of the actual thermal hydraulics code to generate the desired outputs. Since it is a polynomial the computing time for a single code run is reduced from seconds or minutes down to 10^{-3}s. This obviously reduces the computing time necessary and allows for a detailed sensitivity and uncertainty analysis of the specific problem.

Other reductions in computation time can be achieved through the use of parallel and distributed computing or by statistical analysis methods such as Wilk's Method. Wilk's Method reduces the number of simulation runs necessary to obtain a given level of confidence by producing N random samples and then ordering them largest to smallest. The largest value will bound all the other simulations for a given probability γ, and confidence, β. The relation between the number of samples, N, and a given γ and β is defined using Equation 1 for a two sided tolerance and Equation 2 for a single sided tolerance.

$$\beta = 1-\gamma^{N}-(N-1)(1-\gamma)\gamma^{N-1} \ (1), \ \ \beta = 1-\gamma^{N} \qquad (2) \qquad [1]$$

This method has also expanded for use in cases with multiple output variables allowing it to be more useful in the complex systems used in nuclear engineering. For cases with multiple output variables Guba et. al. (2003) defines for a one sided confidence where the number of output variables is defined by p the relation given in Equation 3.

$$\beta = \sum_{j=0}^{N-p} \binom{N}{j} \gamma^{j} (1-\gamma)^{N-j} \qquad (3), \qquad [1]$$

Wilk's method allows for robust analysis with definable statistical benchmarks without the need for the definition of a full response distribution, saving valuable computing time.

Despite the reductions in computing time provided by the aforementioned strategies large computational resources are still required to produce uncertainty and sensitivity analysis with an acceptable level of detail and accuracy. The number of input parameters that can be varied and the various permutations is limited as the more extensive the analysis the much greater the computing demands. Therefore, in most current statistical sampling analysis the list of investigated inputs is small. The analysis is only performed on those inputs deemed to be most important to the simulation output, based on professional experience and engineering judgement. Unfortunately this means that some input parameters which could affect the output are neglected and important portions of the analysis may be missing for new and unfamiliar investigations where there is little data or experience available to evaluate the important input parameters to be modeled. There is an alternative to the sampling methods available in the form of analytical methods which can reduce the simulation time and still provide a robust uncertainty and sensitivity quantification.

2.2 Direct Analytical Methods for Sensitivity Analysis

Direct uncertainty analysis embedded in the code provides sensitivity and uncertainty computations concurrently while the code simulation is running. The equations and numerical methodology of the model is evaluated analytically in order to produce the sensitivity of the model to variations of the input parameters. This method relies on producing the partial derivatives of the model equations for each parameter that can affect the outcome. This method of parallel analysis does require detailed knowledge of the simulation program including all model equations and correlations used down to their base levels. Despite this, once the partial derivations are determined and integrated into the code, the derivatives for each input about any reference value can be computed. This database of partial derivatives can then be utilized separately to perform sensitivity and uncertainty calculations without running the full code. The advantage is that the analytical process of computing partial derivatives need only be done once to assess the relations within the code for any possible transient. In addition, the determination of these partial derivatives provides valuable insight as to which parameters are most important in their affects on the code output. This information will reduce the experience needed and the engineering judgement requirements necessary when establishing which parameters are most important for a specific scenario.

The partial derivatives can be used to develop the output variance and covariance values which are essential to accurate representations of the sensitivity of the system output to its input parameters. If the input parameters are selected and the variation implemented is selected based on experimental uncertainty information a detailed sensitivity analysis is translatable to an uncertainty analysis of the system. By taking the partial derivatives in parallel, a complete set of sensitivities for the full transient can be recorded. This allows the development of concurrent uncertainty calculations which can produce direct upper and lower bounds for a transient. These are very useful in safety analysis and trip assessment to ascertain the realistic state of a system during a transient and determine exact margins to the limits of the scenario. The sensitivity and resulting uncertainty analysis can maintain either a local or global focus. Local analysis examines the interrelations in parameters at a specific local point within the simulation. Therefore, multiple local analyses can be performed to track the sensitivities throughout the simulation both temporally and spatially. Globally focused sensitivity seeks to determine the critical points of the system such as maxima, minima, bifurcations or saddle points.

Direct analytical methods begin with the determination of sensitivities which can then be used to perform uncertainty analysis on the system in question. This is the inverse of statistical methods which begin with uncertainties that can then be developed into a sensitivity evaluation of the system. The direct methods rely heavily on knowledge of the model equations and numerical methods employed within the simulation. If the direct sensitivity analysis procedures are developed in parallel with the construction of the modeling code, the knowledge of the modeling strategies is readily available and the process of integrating sensitivity computations into the modelling code requires minor additional efforts. However, if the modeling code has already been fully developed and there is a desire to modify it to insert direct sensitivity analysis extensive and detailed efforts are required. The modeling code must be fully investigated and dissected to develop an exact understanding as to how the simulation actually functions. The model equations must be explored and traced from high level equations right down to the dependence on the base variables of the system and the input parameters provided by the user. Conversely, the statistical methods tend to treat the code simulation as a black box merely examining the effect of modulating the input parameters on the code outputs. Once the code has been broken down the partial derivatives can be computed from the base level and carried back up the line to the top. When dealing with complex simulation codes such as those used in nuclear thermalhydraulic analyses this process requires considerable time an experience. This is due to the many interacting model equations and extensive lists of parameters utilized within the code.

Despite the extensive understanding required to develop the analytical sensitivity system for direct analysis there are substantial benefits to this method. The computational efforts required to compute the sensitivities and determine consequential uncertainties when dealing with a properly developed parallel sensitivity system is minimal. The sensitivities, once they are known can be used to determine code behaviour for any scenario without requiring extensive sets of full simulation runs. This reduces the computing resources necessary and allows for a more rigorous analysis. The statistical methods require much more computational efforts and must be repeated for any scenario. This huge computing power demand requires that the analysis be limited to only the most important parameters which must be selected using experience and engineering judgement. These selections may be flawed as the simulation code is treated as a black box and its inner workings may severely affect the interaction of parameters that may seem innocuous on the surface. The use of direct analytical methods provides a better understanding of the actual inner workings of the code reducing this need for experience and judgement to define the important parameters. These methods provide detailed evidence on code operation that reduces possible errors arising from improper selection of parameters and promote the full understanding of how the simulation codes function rather than treating them as black boxes.

3. Application of Direct Analytical Methods to Complex Systems

As stated earlier, if direct analytical methods are employed in conjunction with the development of a system simulation code the extra effort needed is minimal. Unfortunately, the standard thermalhydraulics codes used in nuclear analysis were not developed in this manner. Therefore, in order to apply the direct analytical method to these codes efforts must be made to dissect the codes and determine the proper way to integrate the necessary components into the code. For complex full system codes that are in use today this requires significant effort and skill to properly accomplish. Large system thermalhydraulics codes in use in nuclear analysis such as RELAP5, CATHARE and CATHENA have very high levels of complexity and must be carefully examined in order to breakdown the model equations to the level of state variables and user defined input parameters. The RELAP5 thermalhydraulics code is explored here to provide an example of the complexity and the methodologies utilized to breakdown the high level model equations.

RELAP5, like any other complex full system code, is made up of multiple subroutines designed to model various thermalhydraulic phenomenon. The level of complexity present in RELAP5 would necessitate extensive efforts to fully employ direct analytical uncertainty and sensitivity methods throughout all parts of the code. However, it may be feasible to integrate a direct analytical method into a specific subroutine with an acceptable level of effort. This can lead to the development of a defined procedure to employ direct analytical analysis which can then be applied to other subroutines relatively quickly and easily, building the sensitivity system step by step. The structure of RELAP5 is based on two central modules that solve the hydrodynamic and heat structure equations. The information generated by these modules can then be used to propagate the solution through the defined system and to model certain higher level phenomenon in some of the subroutines. Therefore, these modules must be assessed first. The process of applying direct analytical methods to a complex code is defined in Figure 1 and applies to each important model equation or subroutine.

1. Define important model equations to be investigated.
2. Define set of State Variables (**S**) and parameters ($\boldsymbol{\alpha}$) which define the equations.
3. Breakdown the model equations to a level where all components are defined by the state variables or by specific user defined inputs.
4. Perform partial derivatives on base equations for all inputs.
5. Move up the levels of the code taking partial derivatives until the initial model equation is reached.
6. The set of partial derivatives are available to be used with a defined input covariance matrix for sensitivity analysis.
7. Given defined input uncertainties, the sensitivity information can be used to generate real time output uncertainty bands.

Figure 1: Procedure for Direct Analytical Sensitivity Analysis

The process described seems simple but properly dissecting and breaking down the model equations to the level where all components are in terms of the state variables or specific user defined inputs requires considerable skill and effort. In addition, once this is completed taking the partial derivatives for the parental equations within the original high level model is difficult. In the case of RELAP5, to examine the hydrodynamic model one must investigate and breakdown the three sets of conservation equations. These equations for mass, momentum and energy are defined in the numerically convenient form used by RELAP and are broken down in terms of RELAP's set of state variables $\mathbf{S} = \{ P, U_g, U_f, \alpha_g, v_g, v_f, X_n, \rho_b \}$(Pressure, Vapor and liquid internal energy, Vapor Void Fraction, Vapor and liquid velocity, Non-condensable quality and Boron density) [2]. To provide an example of the complexity of these equations the numerically convenient forms of the vapour and liquid energy conservation equations are shown in Figure 2.

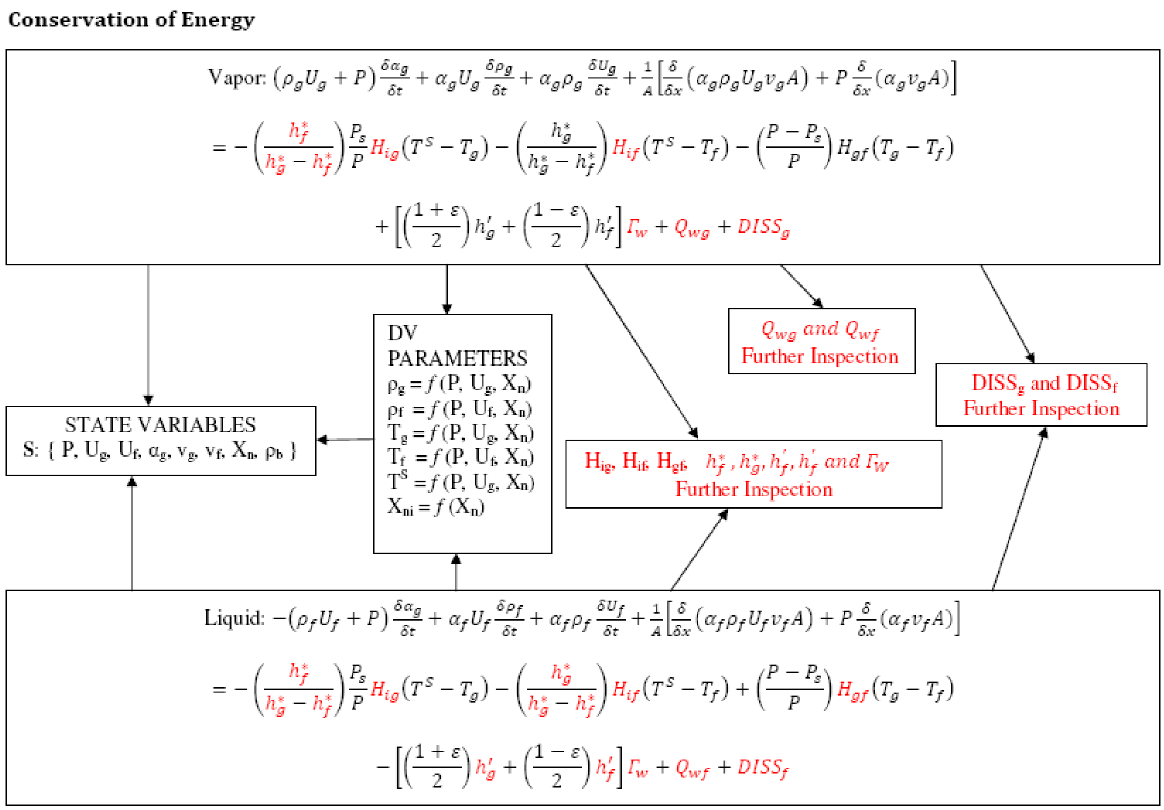

Figure 2: RELAP5Mod3.3 Numerically Convenient Differentials for Conservation of Energy [2]

The equations in Figure 2 are partially broken down to the state variables, some terms (those highlighted in red) require further breakdown to reach the level of state variables or user input parameters. The breakdown of these equations is obviously complex and lengthy and hence is only shown in an abbreviated form here. The breakdown of the equations in RELAP would involve all the hydrodynamic conservation equations which are in some cases several layers deep before the state variables and input parameters are fully reached. Previous work done to apply direct sensitivity methods to thermalhydraulic problems and is explored in the next section.

4. Applications of Direct Sensitivity Analysis to Thermal Hydraulic Systems

Direct analytical sensitivity methods have been applied to several standard thermalhydraulic problems which relate to nuclear engineering. An example is the application by Petruzzi of direct analytical sensitivity analysis through partial derivatives to a simple nitrogen gas blow down system [3]. The system consists of a tank of pressurized nitrogen depressurized into a stagnant air environment at atmospheric pressure. The main properties investigated were the nitrogen pressure transient, the nitrogen temperature and the heat transfer through the tank wall during the blow down. The blow down system equations were explored and converted to discrete form in order to apply a numerical solution code to the problem. The discretized equations were then broken down to the state variables of the system. Once the base level was reached the partial derivatives were taken back up the line until the main model equations were reached.

This relatively simple thermalhydraulic system still retains a high level of complexity. For example the heat transfer coefficient of the nitrogen makes up one component of the nitrogen temperature model equation. The heat transfer coefficient is dependent upon the height, the thermal conductivity and the Nusselt number. At the next level, the Nusselt number is dependent on the Grashof and Prandlt numbers which are in turn dependant on specific nitrogen properties including the density, specific heat capacity, thermal conductivity, dynamic viscosity and gas expansion coefficient. The above nitrogen properties are dependent on temperature and pressure of the gas. Data on nitrogen properties at certain temperatures and pressures is available and usually provided to a simulation code in a tabular format that can be interpolated to provide values for any specific temperature and pressure desired. The parameters affecting the heat transfer include all the nitrogen property values provided in such a table. The partial derivatives of the model equations were determined in terms of all state variables and parameters. This resulted in more than 200 partial derivatives for the nitrogen temperature model alone. It is obvious that even in a simplified system the application of direct analytical methods is arduous. Even so, this endeavour pales in comparison to the number of parameters affecting the model equation of a complex thermalhydraulic code such as RELAP5.

Once the partial derivatives are defined, a covariance matrix of all the inputs is then calculated to be used in conjunction with the partial derivatives to generate a full set of sensitivities for the model equations. Once the set of sensitivities are available they can be utilized in an uncertainty analysis of the code. This process, though lengthy and complex provides detailed sensitivity information for any scenario which the model equations are used to describe. The application of partial derivatives to sensitivity and uncertainty analysis in the described example was performed using both direct derivative conversion and adjoint system operators.

Additional examples of the application of advanced sensitivity analysis tools are available in the theoretical and application work of Cacuci [4]. This includes theoretical development of local and global direct sensitivity analysis, including analytical methods. Applications of the theory are also included providing further insight on how they could be employed to accomplish the process described in Figure 1.

In addition, an explanation of the use of an adjoint system for direct analytical sensitivity analysis is available. For a given operator A, the adjoint operator, A^*, is essentially its conjugate transpose such that the inner product relation, $\langle Ax, y \rangle = \langle x, A^*y \rangle$ holds [4]. The adjoint system is independent of any variations in the original system. The adjoint function that is produced is used to derive the sensitivities of a system response for all system parameters. The adjoint sensitivity equation need only be solved once to obtain the adjoint function and can be solved independently of the original system equation. Once calculated, the adjoint function evaluates the sensitivities of the system response to inputs for any scenario modeled. This method is most useful when the number of parameters exceeds the number of responses being considered. This is the case for many practical application problems and is definitely true for complex thermalhydraulic modelling codes used in nuclear reactor analysis.

5. Progress of Methodology and Future Implementation in RELAP5

The proposed methodology described in Figure 1 seeks to implement direct analytical sensitivity techniques on a subroutine of a common nuclear thermalhydraulic simulation code. The chosen code is RELAP5 and the direct analytic sensitivity will be applied to the choked flow subroutine. This application is an involved and complex undertaking and hence will require much skill and effort over time. The choked flow subroutine derives information from the hydrodynamic and heat structure modules of RELAP so these must also be assessed in the pursuit of the main goal. To refine the process of applying direct analytical sensitivity analysis to a thermalhydraulic simulation and perfect the steps necessary examples such as the simple nitrogen blow down investigated by Petruzzi and the theoretical applications performed by Cacuci are being examined.

Currently, an examination of the application of direct analytical sensitivity methods on simpler problems is being conducted. Resources such as those described in Section 4 are helping to understand the challenges and possible strategies that can be applied. In parallel, the choked flow subroutine and the hydrodynamic and heat structure modules of RELAP5 are being broken down as per step 3 using the RELAP5 code manuals as a roadmap describing the modelling approach. Once this is complete, the relation between the choked flow subroutine and the two modules will be established and the process of taking partial derivatives up the line can commence.

The future implementation work required involves a full review and understanding of possible strategies for the conversion from partial derivatives to sensitivities and uncertainties. Information on this can be gathered from the literature examples in Section 4 and other available sources which are being sought out at this time. Specifically of interest is information on methods to easily compile proper covariance data for the input parameters. Once this investigation is complete, a set of specific steps to arrive at the full sensitivity analysis and progress to the uncertainty analysis can be developed and implemented. This refined process can be applied to the more complex RELAP5 subroutine. The final goal is to achieve a robust sensitivity analysis for the RELAP5 choked flow subroutine. If the efforts in developing uncertainty analysis conversion methods produce a suitable process, they may also be applied to the RELAP5 subroutine.

6. Conclusion

Direct uncertainty and sensitivity analysis is an increasingly vital research area to provide proper assessment of probabilistic best estimate codes. Direct statistical methods do provide sensitivity and uncertainty information but at great computational cost. Only a small number of input parameters can be included in the sensitivity analysis and must be chosen through experience and engineering judgement. The simulation codes are treated as black box systems and the statistical methods must be repeated for each scenario simulated. Direct analytical methods promote detailed investigation of the inner workings of the simulation to produce sensitivity measurements through the use of partial derivatives. Despite the skill and effort required to perform direct analytical methods on complex simulation codes, the method is only required once to cover all scenarios that the code is able to simulate. This greatly reduces the computational efforts necessary. In addition, the detailed sensitivities derived from this process provide valuable information which can be used to properly rank the inputs in terms of their importance. This reduces the experience and engineering judgement necessary and allows assessment of unexplored scenarios where experience is lacking. By integrating a direct analytical sensitivity method into the simulation code, consistent analysis is made available to all users and a wealth of sensitivity information is provided. This information can also be utilized to produce real time uncertainty analysis which is of great value to the determination of realistic plant operation and safety analysis.

A process for applying direct analytical sensitivity analysis to a complex nuclear thermalhydraulics code is being developed. Reviews of literature describing the application of direct analytical methods to thermalhydraulic problems are being utilized to refine and perfect the process. Once properly established, the procedure will then be applied to the choked flow subroutine of the RELAP5 thermalhydraulics code. The goal will be to arrive at a detailed set of parameter sensitivity values for the choked flow subroutine. These sensitivities could possibly be utilized to perform a real time uncertainty analysis. If successful, the process could be applied to other subroutines helping to contribute to a full code sensitivity analysis.

7. References

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