HIGHER ORDER ACCURATE K-EIGENVALUE SENSITIVITY ESTIMATION USING THE COMPLEX-STEP DERIVATIVE METHOD

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ABSTRACT

This paper employs the complex-step derivative method (CDM) to calculate the *k*-eigenvalue sensitivity with respect to nuclear cross-section in reactor applications. The CDM utilizes a Taylor series expansion in the complex-plane whereby the imaginary part of the complex solution space represents the gradient. This numerical approach offers many advantages over conventional techniques such as first-order perturbation theory. A one-group one-dimensional *k*-eigenvalue problem is used in the paper as a numerical example to demonstrate the feasibility of the CDM in reactor problems. The preliminary results from the numerical example justify the viability and higher accuracy of the CDM through a one-to-one comparison to the results from the direct perturbation approach.

KEYWORDS: Sensitivity, Complex-step Derivative Method, *k*-eigenvalue problem

1. INTRODUCTION

Sensitivity analysis investigates the variation of the outputs of a system to changes in the input parameters. The commonly used formulations for sensitivity analysis use approaches that result in only first-order approximation to gradient calculations. These numerical approaches typically restrict the permissible perturbation range of the sensitivity parameter and may possess significant variability between functions of interest and selected parameters. Therefore, sensitivity estimation that possesses higher accuracy is required to enable a larger perturbation range of the input parameter. Furthermore, computing these sensitivities with higher accuracy will benefit many aspects in the system design procedure and facilitate optimization and scoping studies of the system. The work presented in this paper intends to obtain highly accurate sensitivities of the system using a complex-variable based derivative estimation approach. This approach was originally pioneered in [1] for the computation of sensitivity derivatives, and revisited in the literature by numerous researchers, such as [2].

The standard computational approaches employed to solve the neutron transport equation (which is the primary mathematical model for nuclear reactor calculations) involve a sophisticated nestled iteration paradigm due to the inherent complexity of the equation. It is likely owning to this sophisticated iteration procedure, the existing transport solver cannot generate correct answers if it is loaded with complex inputs directly. Due to this reason, special treatment must be exercised in the transport solver to make it capable of handling the complex variable approach. Section 3 gives a detailed description of this treatment to the neutron transport model for the purpose of implementing the complex variable derivative approach in the model to enable complex-derivative method to evaluate the sensitivity.

2. SENSITIVITY ANALYSIS AND DERIVATIVE COMPUTATIONS

2.1. Sensitivity Analysis

In general, any function of interest may be expressed in functional form as $f(x,Q(x))$. Here, it is assumed that the function may have explicit as well as implicit, $Q(x)$, dependencies on the parameter x. For the implicit dependency, the functional form of $Q(x)$ typically is not known and represents the solution to a disciplinary state equation. Hence, Q is often referred to as the disciplinary state vector. In reactor calculations, for example, the effective multiplication factor k_{eff} is the general function f, the nuclear data (i.e., cross-sections) are the implicit parameter x, and the flux is akin to the implicit state vector $Q(x)$.

The sensitivity derivatives of the general function may be obtained by direct differentiation with respect to implicit and explicit dependencies as

$$\frac{df}{dx} = \frac{\partial f}{\partial x} + \left(\frac{\partial f}{\partial Q} \right)^T \frac{\partial Q}{\partial x}. \tag{1}$$

To compute the sensitivity derivative from Eq.(1) the sensitivity of the state vector, $\partial Q/\partial x$, is needed. This approach to sensitivity analysis is referred to as the forward sensitivity analysis procedure (FSAP). Depending on the number of functions of interest that is desired and the number of parameters or independent variables in which sensitivity information is required, a more efficient alternative approach may be formulated. This method is referred to as the adjoint sensitivity analysis procedure (ASAP) [3], and may be written as

$$\frac{df}{dx} = \frac{\partial f}{\partial x} - \lambda_f^T \left[\frac{\partial R}{\partial x} \right], \tag{2}$$

where λ_f are adjoint vectors defined in such a way as to eliminate the dependence of the functions on the sensitivity of the state vector. As discussed below, R represents the disciplinary state equations.

For the FSAP, Eq.(1), the sensitivity of the state vector $\partial Q/\partial x$ is required, and for the ASAP, Eq.(2), the adjoint vectors λ_f are needed. To obtain these, the state equation, which may be generally defined as a residual vector R, can be written symbolically as

$$R(x,Q(x)) = 0, \tag{3}$$

where the explicit and implicit dependencies of the residual on the state vector Q and the parameter of interest are asserted. In the FSAP, Eq.(3) is directly differentiated with respect to the independent variables to produce the following *linear* equation

$$\frac{dR}{dx} = \frac{\partial R}{\partial x} + \frac{\partial R}{\partial Q}\frac{\partial Q}{\partial x} = 0 \tag{4}$$

or, rearranging

$$\frac{\partial R}{\partial Q}\frac{\partial Q}{\partial x} = -\frac{\partial R}{\partial x} \tag{5}$$

where $\partial R/\partial Q$ is the Jacobian matrix evaluated with the state vector given the current value of the parameter of interest.

ASAP begins by combining Eq.(4) from the direct differentiation method with the sensitivity derivatives in Eq.(1). From this adjoint vectors may be conveniently defined such that the sensitivity of the state vector is no longer needed. Nevertheless, the end result requires the solution of the following *linear* system for the adjoint vectors

$$\left(\frac{\partial R}{\partial Q}\right)^T \lambda_f = \frac{\partial f}{\partial Q} \tag{6}$$

Solving for the sensitivity of the state vector in Eq.(5), or for the adjoint vector in Eq.(6), is made more tractable when the above equations are recast into what has been referred to as the incremental iterative form [4, 5]. Omitting details for brevity, using the incremental iterative form, higher-order spatially accurate sensitivity analysis procedures have been developed for shape design optimization of aerodynamic [6-8] and hydrodynamic vehicles [9], acoustic metamaterials [10], and electromagnetic metamaterials [11], among many other application domains. It should be noted that the literature with regards to sensitivity-based shape design optimization is extensive and beyond the scope of the current paper. However, an earlier concise review on the use of sensitivity analysis in shape design optimization has been reported in [12], and the reader is directed to this source for a more detailed discussion of methods presented thus far.

2.2. Derivative Calculations

As seen from the discussion above, the main computation effort required in the sensitivity calculation is to estimate the derivative of the response of interest to the parameter of sensitivity analysis interest. For illustration, assume $f(x)$ is a general response function that is under investigator's interest, the essence of calculating the sensitivity of $f(x)$ with respect to a variable x is to calculate the derivative of $f(x)$ at x. The task of constructing exactly or analytically all of the required linearizations and derivatives by hand for either the FSAP or ASAP, and then building the software for evaluating these terms can be extremely tedious. One solution to this problem has been found in the use of a technique known as automatic differentiation (AD). For this purpose, a pre-compiler software tool, called ADIFOR [13], has been utilized with much success to obtain complicated derivatives from advanced simulation and grid generation codes [14,15].

The AD approach requires differentiation of the simulation software, either by hand or with pre-compiler software. Other methods to obtain sensitivity derivatives are based on numerical techniques. The simplest numerical technique is the finite-difference approximation. Another is a numerical technique that was pioneered by Newman, Anderson, and Whitfield [1, 16-18] for evaluating the derivatives of real functions

with explicit and implicit dependencies on the independent variable and that require the iterative solution to couple nonlinear systems of equations. The technique, which referred to herein as the complex-step derivative method (CDM) has been given various names in the literature, such as the Complex Taylor Series Expansion method among others. In the aforementioned cited literature, this method was demonstrated via the computation of aerodynamic, structural, and multidisciplinary sensitivity derivatives with respect to independent variables appropriate for both aerodynamic and structural design optimizations. Subsequently, the work of Ref. [1] was extended to obtain sensitivity derivatives for turbulent flows by Anderson et al. [17]. Furthermore, this technique is commonly used for linearization and Jacobian evaluation in implicit schemes that involve complicated flux functions. As testament to the ease of implementation, and accuracy of the approach, the method pioneered originally in [1] for sensitivity analysis has been widely adopted and exploited by many researchers at various universities and government laboratories. A complete list of references is extensive and prohibitive to include within the current work. However, for comparison, both numerical approaches noted above will be briefly discussed for below for demonstrative purposes.

The finite-difference approximation to the derivative can be derived to have a desired truncation error. For a first-order approximation to the derivative one may expand the function in a Taylor series about a given point using a forward or a backward step. For example, a forward finite-difference method (FDM) for approximating the derivative may be written as

$$\frac{df}{dx} = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}\frac{d^2 f}{dx^2} + \cdots \tag{7}$$

which has a truncation error of $\mathrm{O}(h)$. To achieve a second-order accurate approximation to the derivative, forward and backward finite-difference approximations may be combined to yield the central finite-difference approximation

$$\frac{df}{dx} = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!}\frac{d^3 f}{dx^3} + \cdots \tag{8}$$

This expression for the derivative has a truncation error of $\mathrm{O}(h^2)$. The advantage of using the finite-difference approximation to obtain sensitivity derivatives is that any existing code may be used without modification. The disadvantages of this method are the computational time required and the possible inaccuracy of the derivatives. The former is due to the fact that for each parameter or independent variable, to obtain second-order accuracy, three evaluations of the function of interest are required for each parameter to evaluate the central finite-difference. In cases where the function evaluations are computationally intensive, these may become prohibitively expensive for a large number of independent variables. For first-order accuracy, only two evaluations are required for either the forward or backward finite-difference approach, and it is usually adopted for computationally demanding analyses. Inaccuracies in the derivative approximations are attributed to the choice of step size. To minimize the truncation error one selects a smaller step size, however, an exceedingly small step size may produce significant subtractive cancellation errors. The optimal choice for the step size is not known a priori, and may vary from one function to another, and from one parameter to the next.

Instead of the finite-difference approximation, consider expanding the function in a Taylor series using a complex step as

$$f\left(x+hi\right)=f\left(x\right)+hi\frac{df}{dx}-\frac{h^2}{2!}\frac{d^2f}{dx^2}-\frac{h^3i}{3!}\frac{d^3f}{dx^3}+\frac{h^4}{4!}\frac{d^4f}{dx^4}+\cdots \tag{9}$$

where $i=\sqrt{-1}$. Solving this expression for the imaginary part of the function yields

$$\frac{df}{dx}=\frac{\mathrm{Im}\left[f\left(x+hi\right)\right]}{h}+\frac{h^2}{3!}\frac{d^3f}{dx^3}-\frac{h^4}{5!}\frac{d^5f}{dx^5}+\cdots \tag{10}$$

This expression for the derivative also has a truncation error of O(h^2). Evaluating the function with a complex argument, both the function and its derivative are obtained simultaneously, without subtractive terms, and thus cancellation errors avoided. The real part is the function value to second order. This method is based on ideas that where explored over five decades ago by Lyness and Moler [19], which demonstrated the use of complex variables to extract derivatives from simple explicit functions (e.g., $x^{9/2}$ and $e^x/(\sin^3 x+\cos^3 x)$).

The advantages of the CDM are numerous. First, like the finite-difference approximation to the derivatives, very little modification to the software is required. All the original features and capabilities of the software are retained. Thus, user experience is not lost and ongoing advancements and enhancements can be readily introduced into subsequent versions without extensive modifications or re-differentiation. This is in direct contrast to hand or automatically differentiated sensitivity analysis codes, where any modification to the original software will require re-differentiation. This advantage is extremely useful in the problem formulation stages when new functions and dependencies are being explored. Second, this method is equivalent to a discrete-direct approach, either from automatic differentiation or hand differentiated codes, in the way that the state vector and its derivatives are being solved for simultaneously. When solving the state equation, the state vector resides in the real part and the derivatives in the imaginary part. Unlike the finite-difference approximation, fully converged evaluations of the state equation are not required to obtain derivatives of sufficient accuracy for analysis. Third, since each complex perturbation is independent, the CDM is ideally suited for parallel computing architectures. Finally, the CDM is not sensitive to step size selection and only requires step sizes that avoid excessive truncation error; thus, it has been shown that this method demonstrates true second-order accuracy [1, 16-18]. Additionally, the CDM technique [see Eq.(9)] can be used, at little to no additional computational costs, to approximate second-derivative information using available data as

$$\frac{d^2f}{dx^2}=\frac{2\left(f\left(x\right)-\mathrm{Re}\left[f\left(x+hi\right)\right]\right)}{h^2}+\mathrm{O}\left(h^2\right) \tag{11}$$

which, like the first-derivative, has second-order truncation error. As can be observed the approximations to the second-derivatives are subject to subtractive cancellation errors and, thus, step-sizes must be selected judiciously.

To demonstrate the aforementioned salient features of the CDM in estimating derivatives with higher accuracy than the FDM a simple analytic example is considered. The partial derivatives of the two variable function $f(x,y)=3x^3+4x^5y^3$ at a certain point can be numerically produced using FDM and CDM by perturbing the variable (x or y) with arbitrarily amount of the values at the point. The results generated using the FDM and CDM with different perturbations are illustrated in Fig. 1. As a reference solution, the exact partial derivatives at the point (x = 3, y =1.5) is also shown in the figure.

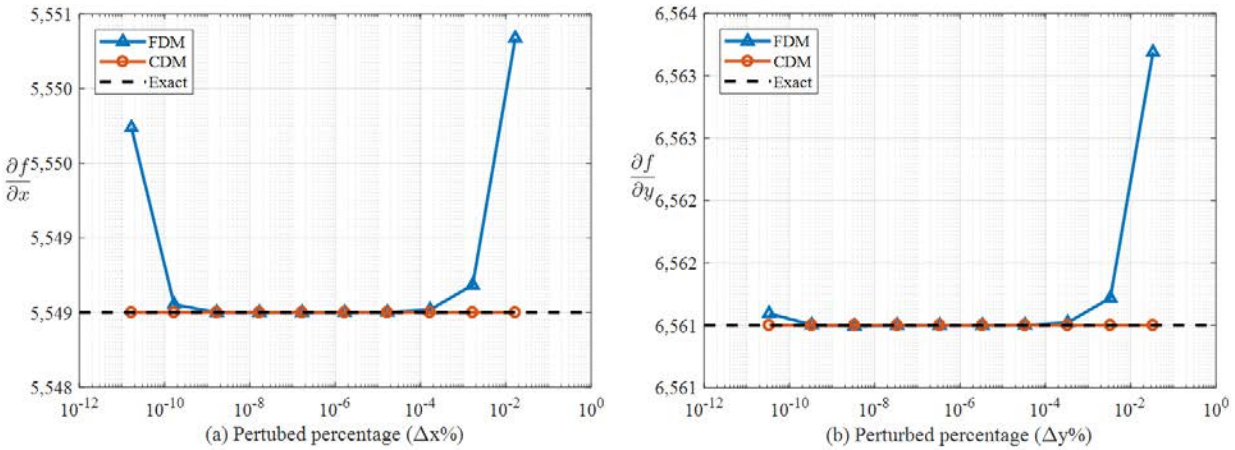

Figure 1. The partial derivative estimate for the function $f(x,y) = 3x^3 + 4x^5y^3$ at x = 3, y =1.5.

As shown in Fig. 1, the results yielded from the FDM deviate from the exact solution when either the step size is large or small. This observation illustrates that when the step size is large the truncation error with respect to the FDM dominate, whereas when the step size is very small the subtractive cancelation errors pollute the derivative approximation. As a contrast, the results yielded from CDM demonstrate that for this explicit function the second-order approximation accurately approximates the derivatives over the perturbations examined and that the approximation is not subjected to subtractive cancellations errors. It should be noted that the current analytic example is based on a benign two variable, explicit function. As such, the perturbation range over which the FDM gives acceptable results for both variables is substantial. This is not typically the case, particularly when implicit dependencies that require the iterative solution to nonlinear state equations are required for the function evaluations. In these cases, there may only exists a very small perturbation range that produces an acceptable derivative approximation, and this range could be different for each function of interest and parameter combination. The CDM method, as described above and found in the cited literature, has been demonstrated not to suffer from these short-comings and is step-size independent, regardless of function or parameter selection.

3. CDM IMPLEMENTATION IN THE *k*-EIGENVALUE TRANSPORT PROBLEM

With standard notations, the one-group one-dimensional *k*-eigevalue neutron transport problem with an isotropic scattering source and uniform materials may be described as the following equation

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \Sigma_t\psi(x,\mu) = \frac{1}{2}\Sigma_s\phi(x) + \frac{1}{2}\frac{\nu\Sigma_f\phi(x)}{k} \quad . \tag{12}$$

If we define the fission source

$$S_f = \nu\Sigma_f\phi(x)\,, \tag{13}$$

Eq.(12) is reduced to

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \Sigma_t\psi(x,\mu) = \frac{1}{2}\Sigma_s\phi(x) + \frac{1}{2}\frac{S_f}{k}\,. \tag{14}$$

In the FDM based derivative calculation, the forward transport solution is first computed to calculated the reference *k*-eigenvalue, denoted as k_0. Then the sensitivity parameter of interest, for example the fission

cross section, is perturbed with a small scale $\Sigma_f' = \Sigma_f(1+h)$. The perturbed *k*-eigenvalue, denoted as k_p, can be computed with the perturbed cross section. Therefore the *k*-eigenvalue sensitivity is approximated by the FDM

$$\left(\frac{\Sigma_f}{k}\frac{\partial k}{\partial \Sigma_f}\right)_{\text{FDM}} = \frac{\Sigma_f}{k}\frac{k_p - k_0}{\Delta\Sigma_f} = \frac{k_p - k_0}{k \cdot h} \ . \tag{15}$$

As can be seen, to obtain the sensitivity information, two forward calculations are required in the FDM.

To enable the complex variable calculation in the transport equation, we consider the following quantities consisting of both real and imaginary parts of the solution space

$$\begin{aligned}
&\psi = \psi_r + \psi_i i \\
&\phi = \phi_r + \phi_i i \\
&\Sigma_t = \Sigma_{t,r} + \Sigma_{t,i} i \\
&\Sigma_s = \Sigma_{s,r} + \Sigma_{s,i} i \\
&k = k_r + k_i i \\
&\nu\Sigma_f = \nu\Sigma_{f,r} + \nu\Sigma_{f,i} i \\
&S_f = S_{f,r} + S_{f,i} i
\end{aligned} \ . \tag{16}$$

By substituting Eq.(16) into Eq.(14), we get

$$\mu\frac{\partial}{\partial x}\left(\psi_r + \psi_i i\right) + \left(\Sigma_{t,r} + \Sigma_{t,i} i\right)\left(\psi_r + \psi_i i\right) = \frac{1}{2}\left(\Sigma_{s,r} + \Sigma_{s,i} i\right)\left(\phi_r + \phi_i i\right) + \frac{1}{2}\frac{S_{f,r} + S_{f,i} i}{k_r + k_i i} \ . \tag{17}$$

With the definitions in Eq.(16), the fission source can be expressed as

$$\begin{aligned}
S_f &= S_{f,r} + S_{f,i} i \\
&= \left(\nu\Sigma_{f,r} + \nu\Sigma_{f,i} i\right)\left(\phi_r + \phi_i i\right) \\
&= \left(\nu\Sigma_{f,r}\phi_r - \nu\Sigma_{f,i}\phi_i\right) + \left(\nu\Sigma_{f,r}\phi_i + \nu\Sigma_{f,i}\phi_r\right) i
\end{aligned} \ . \tag{18}$$

Thus we get

$$\begin{aligned}
S_{f,r} &= \nu\Sigma_{f,r}\phi_r - \nu\Sigma_{f,i}\phi_i \\
S_{f,i} &= \nu\Sigma_{f,r}\phi_i + \nu\Sigma_{f,i}\phi_r
\end{aligned} \ . \tag{19}$$

We process the fission source term in Eq.(17) as follows

$$\frac{1}{2}\frac{S_{f,r}+S_{f,i}i}{k_r+k_i i}=\frac{1}{2}\frac{1}{k_r{}^2+k_i{}^2}\left(k_r-k_i i\right)\left(S_{f,r}+S_{f,i}i\right)$$
$$=\frac{1/2}{k_r{}^2+k_i{}^2}\left(k_r S_{f,r}-k_i S_{f,r}i+k_r S_{f,i}i+k_i S_{f,i}\right)$$
$$=\frac{1/2}{k_r{}^2+k_i{}^2}\left(k_r S_{f,r}+k_i S_{f,i}\right)+\frac{1/2}{k_r{}^2+k_i{}^2}\left(k_r S_{f,i}-k_i S_{f,r}\right)i$$

By equaling the real and imaginary portion of the equation, we get the following two coupled equation for real and imaginary flux solution ψ_r, ψ_i, respectively

$$\begin{aligned}\mu\frac{\partial\psi_r}{\partial x}+\Sigma_{t,r}\psi_r-\Sigma_{t,i}\psi_i&=\frac{1}{2}\left(\Sigma_{s,r}\phi_r-\Sigma_{s,i}\phi_i\right)+Q_{f,r}\\ \mu\frac{\partial\psi_i}{\partial x}+\Sigma_{t,r}\psi_i+\Sigma_{t,i}\psi_r&=\frac{1}{2}\left(\Sigma_{s,r}\phi_i+\Sigma_{s,i}\phi_r\right)+Q_{f,i}\end{aligned}\quad , \tag{20}$$

where

$$\begin{aligned}Q_{f,r}&=\frac{1/2}{k_r{}^2+k_i{}^2}\left(k_r S_{f,r}+k_i S_{f,i}\right)\\ Q_{f,i}&=\frac{1/2}{k_r{}^2+k_i{}^2}\left(k_r S_{f,i}-k_i S_{f,r}\right)\end{aligned}\quad . \tag{21}$$

With the calculation of the imaginary portion of the *k*-eigenvalue (i.e., k_i), the *k*-eigenvalue sensitivity estimation by the CDM can be obtained as follows

$$\left(\frac{\Sigma_f}{k}\frac{\partial k}{\partial\Sigma_f}\right)_{\text{CDM}}=\frac{\Sigma_f}{k}\frac{k_i}{\Sigma_f\cdot h}=\frac{k_i}{k\cdot h}\ . \tag{22}$$

where $\Sigma_f h=\Sigma_{f,i}$ is the designated imaginary portion of the fission cross-section in the complex solution calculation. As seen in Eq.(20), the CDM need to perform two forward calculations to estimate one sensitivity value, which implies the computation efforts spent in the CDM is identical to the one in FDM.

4. NUMERICAL RESULTS

For demonstration purposes, a multi-region 1D slab geometry reactor is used as an example. This geometry consists of three regions: 4, 8, 4 cm in regions 1 through 3, respectively. Vacuum conditions are assumed for both sides of the slab. A *k*-eigenvalue problem is constructed using the materials given in Table I. The reference *k*-eigenvalue for this multiplying system is 1.38478. The one-group one-dimensional transport equation was numerically solved by the discrete ordinate method (i.e., S_N). Standard diamond difference scheme is used for the spatial discretization. For this oversimplified example, no negative flux is observed, thus no zero-fixed approach is applied in the code. Source iteration is performed for the flux convergence and power iteration is operated to pursue the *k*-eigenvalue convergence. For all the calculations, S_6 quadrature set and an uniform small mesh size of $\Delta x=0.2$ cm were used to minimize the numerical truncation errors due to angular and spatial discretizations.

Table I. Material Properties of the Numerical Example.

	Region 1	Region 2	Region 3
Σ_t [cm^{-1}]	0.2	0.75	0.3
Σ_s [cm^{-1}]	0.15	0.01	0.2
$\nu\Sigma_f$ [cm^{-1}]	0.1	0.8	0.2

Following the methodologies described in Section 3, the derivatives of k-eigenvalue with respect to the cross sections for FDM and CDM were calculate and compared as shown in Fig. 2. Note the parameter is perturbed with different percentage amount from 100% to 0.1% for both methods. As seen in Fig. 2, the *k*-eigenvalue sensitivity results exhibit a similar behavior pattern as shown in Fig. 1 for the simple analytic function case. The advantageous features of the CDM are clearly verified by these results. For both derivatives, the FDM can arrive at the correct solution when the perturbation range is restricted to ~1%. The CDM can go beyond the perturbation limit remarkably, the correct derivative value can be produced even for the case the perturbation range reaches 100%.

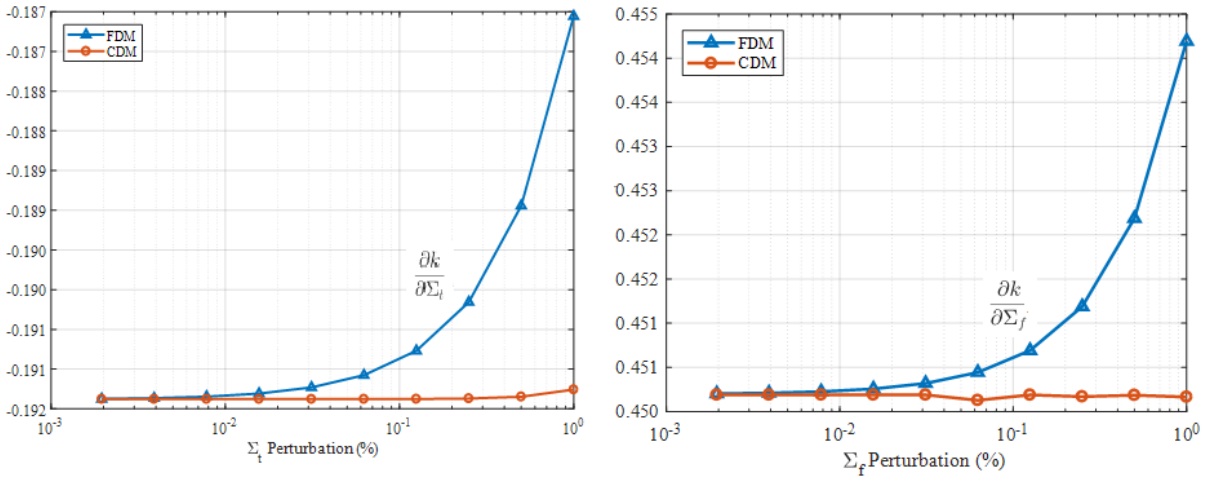

Figure 2. The comparison of *k*-eigenvalue derivative with respect to the total cross section (left) and fission cross section (right) with the FDM and CDM.

5. CONCLUSIONS AND FUTURE WORK

The complex-step derivative method is developed and applied in neutron transport models to calculate the *k*-eigenvalue sensitivity with respect to nuclear cross-section. The CDM utilizes a Taylor series expansion in the complex-plane whereby the imaginary part of the complex solution space represents the gradient. The feasibility of the CDM method is demonstrated with a one-group one-dimensional *k*-eigenvalue problem. The higher order accuracy of the derivative estimation by CDM is justified by comparing the result obtained from the conventional first-order finite difference method. Future efforts on this work will be extending the current transport model to a multi-group multi-region problem, and demonstrate the advantages of CDM in adjoint sensitivity analysis, as well as handling non-linear effects in the sensitivities.

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