Higher Order Accurate *k*-eigenvalue Sensitivity Estimation Using the Complex-step Derivative Method

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Introduction

- Sensitivity analysis investigates the variation of the outputs of a system to changes in the input parameters
- Most commonly used formulations for sensitivity analysis limit in the first-order approximation
- Higher order accurate sensitivities are desirable in many applications
- Complex-step Derivative method (CDM) can be used to compute higher order accurate sensitivities

Sensitivity Analysis

- Express a general function of interest as $f(x, Q(x))$, where x is the parameter and $Q(x)$ is the state variable.
- Forward Sensitivity Analysis Procedure (**FSAP**)

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

- Adjoint Sensitivity Analysis Procedure (**ASAP**)

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

where R is the state equation and λ_f^T is adjoint vector.

Derivative Calculations

- For either FSAP or ASAP, the essential task in sensitivity analysis is to obtain sensitivity **derivatives**.
- Finite Difference Method (**FDM**)

$$\left(\frac{df}{dx}\right)_{\mathrm{FDM}} \approx \frac{f(x+h)-f(x)}{h}$$

- Taylor series analysis informs FDM only has the **first-order** accuracy:

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

Complex-step Derivative Method (CDM)

- To introduce **CDM**, performing the Taylor series expansion to a function of ***complex variable*** as follows

$$f(x+ih)=f(x)+ih\frac{df}{dx}-\frac{h^2}{2}\frac{d^2f}{dx^2}-i\frac{h^3}{3!}\frac{d^3f}{dx^3}+o(h^3)$$

- Take the imaginary part of the equation

$$\mathrm{Im}[f(x+ih)]=h\frac{df}{dx}-\frac{h^3}{3!}\frac{d^3f}{dx^3}+o(h^3)$$

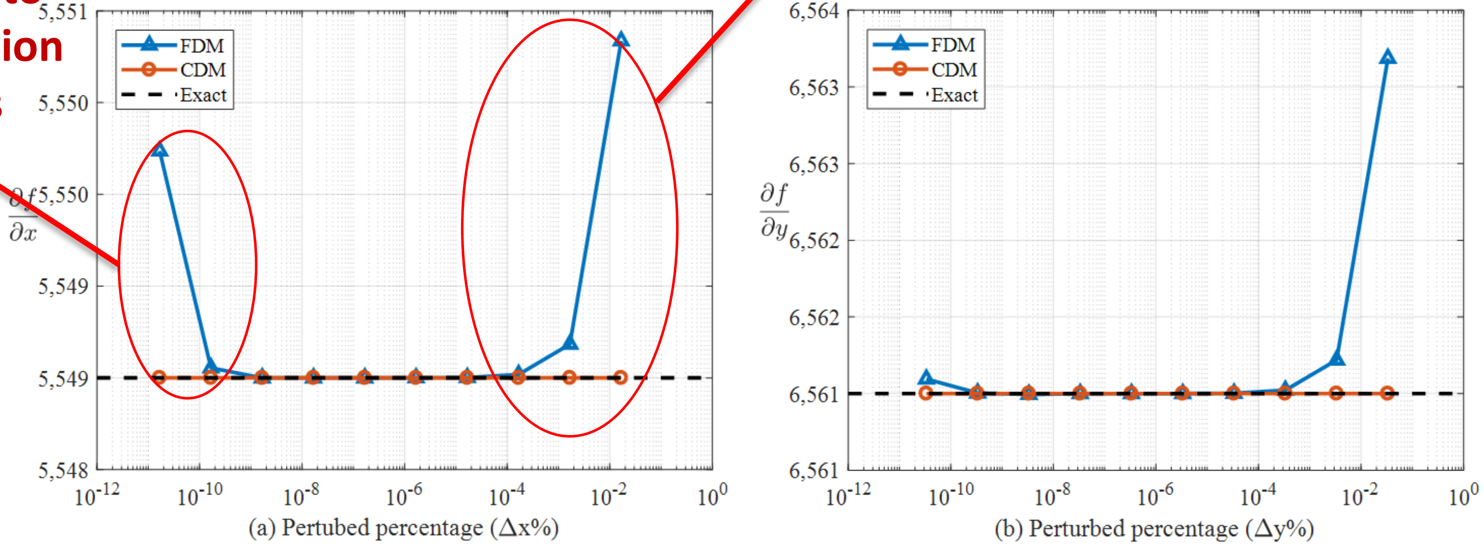
- This gives the CDM derivative estimation

$$\left(\frac{df}{dx}\right)_{\mathbf{CDM}}=\frac{\mathrm{Im}[f(x+ih)]}{h}+\frac{h^2}{3!}\frac{d^3f}{dx^3}+o(h^2)$$

A Simple Example

Bounded by the first-order accuracy

Subject to cancellation errors



The partial derivatives estimated for $f(x, y) = 3x^3 + 4x^5y^3$ at $x = 3$, $y = 1.5$.

Nested Iterative Hierarchy for *k-eigenvalue Solver*

Start of program

*Begin of the **power iteration** (PI)*

Loop on the energy group g

*Begin of **source iteration** (SI)*

Transport sweep (loop on each direction and each spatial variable)

DSA acceleration if needed

Check SI convergence to decide exit or update and continue

End of SI

End of the energy group loop

Check PI convergence to decide exit or update and continue

End of the PI

End of program

Challenges of CDM in *k*-eig Sensitivity Application

- Standard computational approaches to solve the neutron transport equation involve a sophisticated nestled iteration paradigm due to the inherent complexity of the equation
- Likely due to this reason, the existing transport solver is not compatible with complex inputs
- Special treatment must be exercised in the transport solver to apply complex variable method

CDM Implementation in *k*-eig Transport Problem

- Consider one-group one-dimensional *k*-eig neutron transport problem with an isotropic scattering source and homogeneous materials

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

- With an arbitrary perturbation to the fission cross section $\Sigma'_f = \Sigma_f(1+h)$, for example, the FDM based *k*-eig sensitivity can be estimated

$$\left(\frac{\Sigma_f}{k}\frac{\partial k}{\partial \Sigma_f}\right)_{\mathbf{FDM}} = \frac{\Sigma_f}{k}\frac{k_p - k}{\Delta \Sigma_f} = \frac{k_p - k}{k \cdot h}$$

- To enable the CDM derivative evaluation in the transport solver, we consider the following quantities consisting of both real and imaginary parts of the solution space

$$\psi = \psi_r + \psi_i i, \qquad \phi = \phi_r + \phi_i i$$
$$\Sigma_t = \Sigma_{t,r} + \Sigma_{t,i} i, \qquad \Sigma_s = \Sigma_{s,r} + \Sigma_{s,i} i$$
$$\nu\Sigma_f = \nu\Sigma_{f,r} + \nu\Sigma_{f,i} i, \qquad S_f = S_{f,r} + S_{f,i} i$$
$$k = k_r + k_i i$$

CDM Implementation (cont.)

- Substitute these assumptions into the transport equation, with some arrangements, we arrive at a set of two coupled transport equations counting the real and imaginary portion of the original equation, respectively:

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

$$\mu\frac{\partial\psi_i}{\partial x}+\Sigma_{t,r}\psi_i+\Sigma_{t,i}\psi_r=\frac{1}{2}\left(\Sigma_{s,r}\phi_i+\Sigma_{s,i}\phi_r\right)+Q_{f,i}$$

where

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

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

and

$$S_{f,r}=\nu\Sigma_{f,r}\phi_r-\nu\Sigma_{f,i}\phi_i$$

$$S_{f,i}=\nu\Sigma_{f,r}\phi_i+\nu\Sigma_{f,i}\phi_r$$

- The CDM based *k*-eig sensitivity is thus evaluated by

$$\left(\frac{\Sigma_f}{k}\frac{\partial k}{\partial\Sigma_f}\right)_{\mathrm{CDM}}=\frac{\Sigma_f}{k}\frac{k_i}{\Sigma_f\cdot h}=\frac{k_i}{k\cdot h}$$

where $\Sigma_f h=\Sigma_{f,i}$.

Numerical Example

- **Problem**: a three-region *k*-eigenvalue problem.

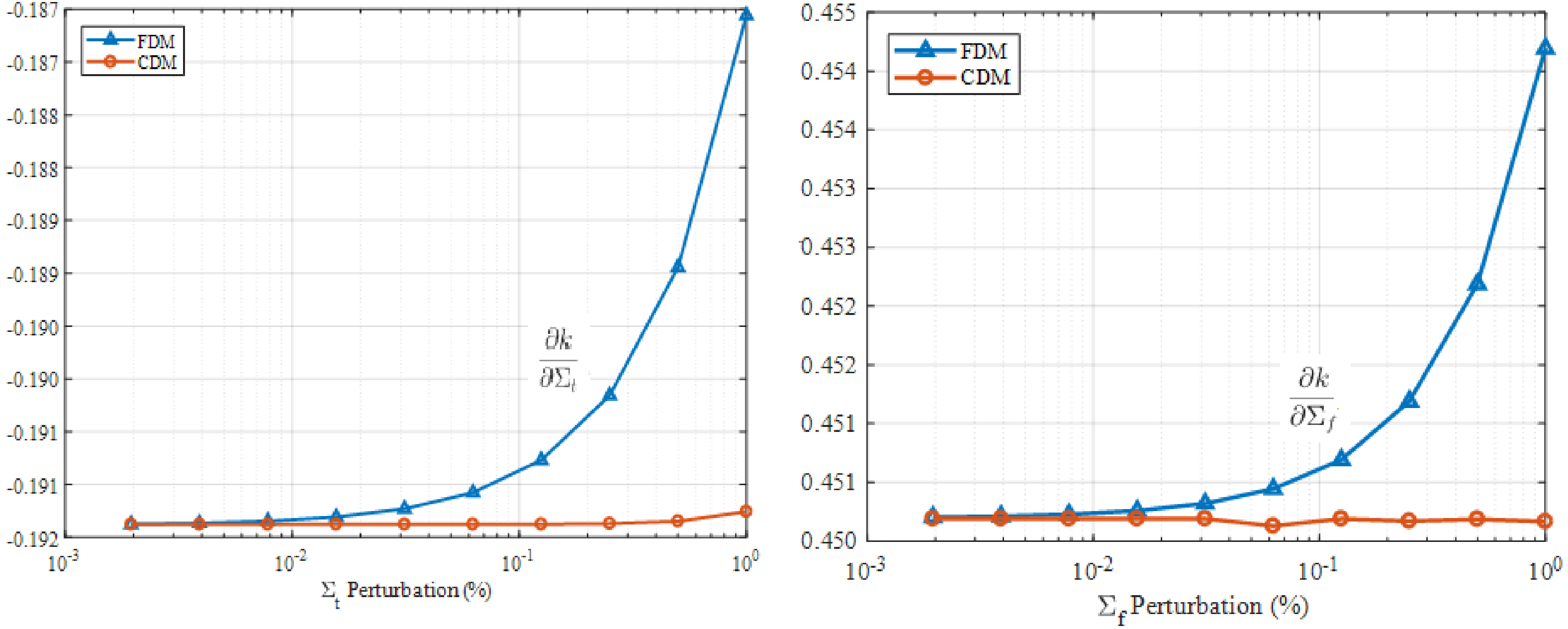
	Region 1	Region 2	Region 3
Σ_t [cm^{-1}]	0.2	0.75	0.3
Σ_s [cm^{-1}]	0.15	0.01	0.2
$\nu\Sigma_f$ [cm^{-1}]	0.1	0.8	0.2
x [cm]	$0 \leq x < 4$	$4 \leq x < 12$	$12 \leq x \leq 16$

- Vacuum boundary applies to both sides of the slab.
- The reference k-eigenvalue for the problem is **1.38478**.

Some Numerical Details

- The 1G 1D transport equation was numerically solved by the **discrete ordinate** method (i.e., S_N method)
- Standard **diamond difference** scheme for the spatial discretization
- **Source iteration** for the flux convergence and **power iteration** for the *k*-eigenvalue convergence
- S_6 Gauss-Legendre quadrature set and uniformly small mesh size **0.2 cm** were used to minimize the numerical truncation errors due to angular and spatial discretizations, respectively

Results



Comparison of *k*-eig derivative to the total cross section (left) and fission cross section (right) with the FDM and CDM

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Summary and Future Work

- The complex-step derivative method (CDM) is developed and applied in neutron transport models to calculate the *k*-eig sensitivity with respect to nuclear cross-section.
- The feasibility of the CDM method is demonstrated with a 1G 1D slab *k*-eig problem. The higher order accuracy of the derivative estimation by CDM is achieved by comparing the result to the first-order finite difference method (FDM).
- Future work will be extending the method to more practical applications (e.g., MG MD heterogeneous problem), and demonstrate the advantages of CDM in adjoint sensitivity analysis, as well as handing non-linear effects in the sensitivities.

Thanks for your time

Questions?