DUAL NUMBER AUTOMATIC DIFFERENTIATION AS APPLIED TO TWO-GROUP CROSS-SECTION UNCERTAINTY PROPAGATION

by

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This work addresses the problem of propagating uncertainty from group-wise neutron cross-sections to the results of neutronics diffusion calculations. Automatic differentiation based on dual number arithmetic was applied to uncertainty propagation in the framework of local sensitivity analysis. As an illustration, we consider a two-group diffusion problem in an infinite medium, which has a solution in a closed form. We employ automatic differentiation in conjunction with the sandwich formula for uncertainty propagation in three ways. Firstly, by evaluating the analytical expression for the multiplication factor using dual number arithmetic. Then, by solving the diffusion problem with the power iteration algorithm and the algebra of dual matrices. Finally, automatic differentiation is used to calculate the partial derivatives of the production and loss operators in the perturbation formula from the adjoint-weighted technique. The numerical solution of the diffusion problem is verified against the analytical formulas and the results of the uncertainty calculations are compared with those from the global sensitivity analysis approach. The uncertainty values obtained in this work differ from values given in the literature by less than 1 10^{-5}.

Key words: automatic differentiation, dual numbers, sandwich formula, sensitivity analysis, uncertainty propagation, power iteration

INTRODUCTION

Sensitivity and uncertainty analysis has become an important topic in nuclear reactor modelling. Uncertainty analysis methods are employed to quantify the effect that the uncertainties in the model input have on the uncertainty of the model output (propagate the uncertainty). Sensitivity analysis is used to study how the uncertainty in the output of a mathematical model can be allocated to different sources of uncertainty in its inputs. Sensitivity and uncertainty analysis methods can be collected into two families, referred to as local and global sensitivity analyses. Local sensitivity analysis methods (the focus of this work) allow one to examine the behaviour of the model output in the vicinity of a chosen point (point of interest). Global sensitivity analysis methods allow one to explore the full phase-space of input parameters, and to take the nonlinearity of the model into account. More detail on sensitivity and uncertainty analysis and their application can be found, for instance in [1].

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Uncertainty propagation in nuclear reactor calculations is typically done using sampling methods or perturbation theory. In sampling methods, a large number of cross-section sets (or libraries) are constructed by sampling from an underlying set of cross-sections and their uncertainties. Calculations are run with all these libraries, and statistical analysis can be performed on the complete set of output parameters obtained. Examples of reactor simulation codes that use this approach are XSUSA [2] and Sampler [3]. The perturbation theory approach involves solving a generalized adjoint equation for each response of interest, to calculate sensitivity coefficients. Uncertainty in responses can then be calculated using the so-called sandwich formula. Examples of codes that use this approach are TSUNAMI [4] and CASMO-4 [5]. These two methods are widely published and not further discussed in this work.

We discuss an alternative approach to uncertainty propagation, based on dual number automatic differentiation and the sandwich formula. Automatic differentiation provides a means for the accurate evaluation of function derivatives in numerical calculations [6-8] by exploiting the fact that derivatives of a

function can be calculated via elementary arithmetic operations (addition, subtraction, multiplication, division) and elementary functions (exp, log, sin, cos, *etc.*) by applying the chain rule repeatedly to these operations [8]. Automatic differentiation requires a small factor more arithmetic operations than an alternative approach, such as finite difference or symbolic differentiation, and is accurate to working precision [9, 10].

In this work, dual number arithmetic is used to implement automatic differentiation. There have been a limited number of papers on the application of automatic differentiation in nuclear engineering, [11-14], and this work is intended to illustrate some relevant concepts, whereas a more detailed description of automatic differentiation can be found, for instance in [13, and references therein].

A common source of uncertainty in reactor calculations is the basic nuclear data libraries and the experimental and modelling uncertainties that they inherently carry [15]. To explore the possibility of employing dual number automatic differentiation for uncertainty propagation in reactor calculations, we study the propagation of uncertainty from broad-group neutron cross-sections to the results of neutronics diffusion calculations. In particular, we will calculate the uncertainty in neutron multiplication factor caused by the uncertainty in broad -group cross-section data.

We demonstrate the approach with a pre-homogenized BWR fuel assembly in two broad energy groups with reflective boundary conditions and assume that cross-section uncertainties have already been propagated through a lattice calculation to the homogeneous broad-group cross-sections. The two-group diffusion problem in infinite medium has a solution in a closed form, that can be used for verification of results obtained with the automatic differentiation, and is a good example on which to demonstrate the concepts involved. Uncertainty propagation results for this problem have been published and can be used for verification [16, 17].

THEORY

In this section dual number arithmetic is described and automatic differentiation within this method is discussed.

Dual number arithmetic

Dual numbers are an extension of real numbers by a second component called the *dual part*. A dual number can be represented in the form [18, 9]

$$\hat{x} \quad x \quad \varepsilon\tilde{x} \tag{1}$$

where x and $\tilde{x}$ are both real numbers and ε – the *dual unit*. The dual unit is analogous to the imaginary unit, $i^2 = -1$, used in complex number arithmetic but defined as $\varepsilon^n \quad 0$ for $n \quad 2$. Numbers x and $\tilde{x}$ are referred to as the *real* (or *primal*) and *dual* parts of $\hat{x}$, respectively. Dual number arithmetic is described with ordinary arithmetic on the primal component and first-order differentiation arithmetic on the dual part. Thus, the basic arithmetic operations are defined as [18]

$$\hat{x} \quad \hat{y} \quad (x \quad \varepsilon\tilde{x}) \quad (y \quad \varepsilon\tilde{y}) \quad (x \quad y) \quad \varepsilon(\tilde{x} \quad \tilde{y}) \tag{2}$$

$$\hat{x}\,\hat{y} \quad (x \quad \varepsilon\tilde{x})(y \quad \varepsilon\tilde{y}) \quad xy \quad \varepsilon(\tilde{x}y \quad x\tilde{y}) \tag{3}$$

$$\frac{\hat{x}}{\hat{y}} \quad \frac{x \quad \varepsilon\tilde{x}}{y \quad \varepsilon\tilde{y}} \quad \frac{x}{y} \quad \frac{\varepsilon(\tilde{x}y \quad x\tilde{y})}{y^2}, (y \quad 0) \tag{4}$$

Functions of dual numbers are introduced via the corresponding Taylor series expansions

$$f(x \quad \varepsilon\tilde{x}) \quad \sum_{n \quad 0}^{\infty} \frac{f^{(n)}(x)\tilde{x}^n\varepsilon^n}{n!} \tag{5}$$

in which all second-order and higher-order terms vanish because $\varepsilon^n \quad 0$ for $n \quad 2$ by the definition, thus yielding

$$f(x \quad \varepsilon\tilde{x}) \quad f(x) \quad f'(x)\tilde{x}\varepsilon \tag{6}$$

As one may observe, the result on the right-hand side of eq. (6) is a dual number, therefore the dual valued function $f(\hat{x}) \quad f(x) \quad \varepsilon\tilde{x}f'(x)$ may be associated with it. Applying eq. (6) to analytic functions provides expressions for the corresponding functions in dual arithmetic. For example, the cosine of a dual argument is defined and evaluated in the following way: $\cos(\hat{x}) \quad \cos(x) \quad \varepsilon\tilde{x}\sin(x)$. A non-comprehensive list of standard analytic functions of a dual number argument can be found in [9, 10].

Equation (6) can be extended to functions of several variables. Recall that for a function h of a vector argument, $\mathbf{x}$, the first two terms of the Taylor series expansion in the vicinity of $\mathbf{x} = \mathbf{x}_0$, are

$$h(\mathbf{x}) \quad h(\mathbf{x}_0) \quad \nabla h(\mathbf{x}_0)\,(\mathbf{x} \quad \mathbf{x}_0) \tag{7}$$

Therefore, a function h of a dual vector argument, $\hat{\mathbf{x}} = \mathbf{x} + \tilde{\mathbf{x}}\varepsilon$, is given by

$$\hat{h}(\hat{\mathbf{x}}) \quad h(\mathbf{x}) \quad \nabla h(\mathbf{x})\,\tilde{\mathbf{x}}\varepsilon \tag{8}$$

where the dual part contains the derivative of the function in the direction of the vector $\tilde{\mathbf{x}}$.

In some applications, one may need to solve a linear problem involving dual numbers. A dual version of basic operations and algorithms of linear algebra exists [18, 9, 10], and those that are used in this study are briefly introduced in the paragraphs that follow.

A dual matrix $\hat{\mathbf{A}}$ is a matrix whose components are dual numbers. It can be split into a real part $\mathbf{A}$ and a dual part $\tilde{\mathbf{A}}$ such that

$$\hat{\mathbf{A}} \quad \mathbf{A} \quad \varepsilon\tilde{\mathbf{A}} \tag{9}$$

The sum and the difference of two dual matrices are therefore given by

$$\hat{\mathbf{A}} \quad \hat{\mathbf{B}} \quad \mathbf{A} \quad \mathbf{B} \quad \varepsilon(\tilde{\mathbf{A}} \quad \tilde{\mathbf{B}}) \tag{10}$$

and the product of two dual matrices is defined as

$$\hat{\mathbf{A}}\hat{\mathbf{B}} \quad \mathbf{AB} \quad \varepsilon(\mathbf{A}\tilde{\mathbf{B}} \quad \tilde{\mathbf{A}}\mathbf{B}) \tag{11}$$

The inverse of a dual matrix (under the convention $\hat{\mathbf{A}}^{-1}\hat{\mathbf{A}} \quad \mathbf{I}+\varepsilon\mathbf{O}$, where **I** and **O** are the real-valued identity and null matrices, respectively) can be calculated in the following way

$$\hat{\mathbf{A}}^{\ 1} \quad \mathbf{A}^{\ 1} \quad \varepsilon\mathbf{A}^{\ 1}\tilde{\mathbf{A}}\mathbf{A}^{\ 1} \tag{12}$$

The norm of dual number vectors is given by

$$\left\|\hat{\mathbf{x}}\right\|_2 \quad \sqrt{\hat{\mathbf{x}}^T\hat{\mathbf{x}}} \tag{13}$$

The determinant, the pseudoinverse, the QR-, Cholesky- and singular value decompositions of a dual matrix, solution of a system of dual linear equations, eigenvalues, and eigenvectors of a dual matrix all are defined and details about them can be found in [18, 9, 10].

Automatic differentiation with dual number arithmetic

It was already mentioned that dual numbers can be used for automatic differentiation. As per eq. (6), the automatic differentiation of a function f at $x \quad \mathbf{R}$ is performed by evaluating $f(x \quad \tilde{x}\varepsilon)$ using dual number arithmetic and choosing $\tilde{x} \quad 1$

$$f(x \quad \varepsilon) \quad f(x) \quad \varepsilon f'(x) \tag{14}$$

From eq. (14) we note that the real part of $f(x+\varepsilon)$ contains the function value at x, and the dual part contains the first derivative of the function, also evaluated at x. The same holds for a multivariate function. The i^{th} component of $f(\mathbf{x})$ at $\mathbf{x} \quad \mathbf{R}^n$ is obtained by evaluating $f(\mathbf{x} \quad \mathbf{e}_i\varepsilon)$, where $\mathbf{e}_i$ is the unit vector in the coordinate direction x_i

$$f(\mathbf{x} \quad \mathbf{e}_i\varepsilon) \quad f(\mathbf{x}) \quad \frac{\partial f}{\partial x_i}\mathbf{e}_i\varepsilon \tag{15}$$

We note here that calculation of all components of the gradient vector requires n function evaluations, however, in many applications only a directional derivative is required and not the gradient, hence only one function evaluation is needed. Furthermore, automatic differentiation using dual number arithmetic leads to no truncation error and no cancellation error as compared to the finite-difference approach [6]. Dual number automatic differentiation corresponds to the so-called forward accumulation (or forward mode) automatic differentiation [8, 13].

In summary, we see that automatic differentiation provides a means for an accurate evaluation of function derivatives in numerical calculations.

UNCERTAINTY PROPAGATION THROUGH AUTOMATIC DIFFERENTIATION

It is rapidly becoming the norm to use the best estimate plus uncertainty calculations for nuclear reactor analysis. Sensitivity and uncertainty analysis can provide useful information on the accuracy and robustness of a model or experimental measurement. There are several methods for sensitivity and uncertainty analysis. This section focuses on the application of dual number automatic differentiation to uncertainty propagation in the framework of local sensitivity analysis.

Uncertainty propagation in the context of local sensitivity analysis

Consider a mathematical model described by a function $\mathbf{R}^n \quad \mathbf{R}$

$$y \quad y(\mathbf{x}) \quad y(x_1,\ldots,x_n) \tag{16}$$

and let $\mathbf{x}_0 = (x_{0,1},\ldots, x_{0,n})$ be a specific point of interest. Linearising the response in the vicinity of $\mathbf{x}_0$ yields

$$y(\mathbf{x}) \quad y(\mathbf{x}_0) \quad \sum_{i\ 1}^{n} \left.\frac{\partial y}{\partial x_i}\right|_{\mathbf{x}\ \mathbf{x}_0} (x_i \quad x_{0,i}) \tag{17}$$

where the partial derivative of the response y with respect to the input x_i (where $i = 1, ..., n$)

$$s_i \quad \left.\frac{\partial y}{\partial x_i}\right|_{\mathbf{x}\ \mathbf{x}_0} \tag{18}$$

can be interpreted as the mathematical definition of the *sensitivity* of y with respect to x_i at $\mathbf{x}_0$. By collecting sensitivities s_i to a sensitivity vector, $\mathbf{s} \quad y(\mathbf{x}_0) \quad (s_1,\ldots,s_n)$, eq. (17) can be written in a vector form

$$\begin{aligned} y(\mathbf{x}) \quad y(\mathbf{x}_0) \quad & y(\mathbf{x}_0)\ (\mathbf{x} \quad \mathbf{x}_0) \\ & y(\mathbf{x}_0) \quad \mathbf{s}\ (\mathbf{x} \quad \mathbf{x}_0) \end{aligned} \tag{19}$$

Now, let us assume that $\mathbf{x}$ is a random vector with a known mean, $\boldsymbol{\mu} = E[\mathbf{x}] = (\mu_1,\ldots,\mu_n)$, and uncertainty described by the covariance matrix $\mathbf{C} = E[(\mathbf{x}-\boldsymbol{\mu} \quad \mathbf{x}-\boldsymbol{\mu}$, where the symbol "$T$" denotes the matrix transpose. The uncertainty of the response is characterized by its variance and can be computed for the linearised response by applying the so-called *sandwich rule* [1]

$$\mathrm{var}[y] \quad \mathbf{s}^T\mathbf{Cs} \tag{20}$$

In practice, one can assume that the covariance matrix **C** is given, and the challenge is to calculate the sensitivity vector **s**.

Application of dual number automatic differentiation

We will use dual number arithmetic to calculate the uncertainty of function y. Consider, as before, a function (given analytically or as a computational algorithm)

$$y \quad f(\mathbf{x}) \tag{21}$$

Explicit use of sandwich formula. The simplest, and most straightforward approach to uncertainty propagation would be to first calculate all the components of the sensitivity vector, s_i, by applying eq. (15) n times. The uncertainty is then obtained via the matrix multiplication in the sandwich formula, eq. (20). This approach requires, therefore, n evaluations of dual-valued function $f(\hat{\mathbf{x}})$, as well as one matrix-vector and one vector-vector multiplication.

Implicit use of sandwich formula. Alternatively, one may observe that in eq. (20) the dot product of the sensitivity vector with any row of the covariance matrix (or column, due to the symmetry of covariance matrices) is the derivative in the direction defined by this row (or column). Let $\mathbf{c}_i$ be the i^{th} row of the covariance matrix of inputs, $\mathbf{C}$, where $i = 1,\ldots,n$. We use the dual number arithmetic to evaluate n auxiliary quantities at given $\mathbf{x}_0$

$$\hat{z}_i \quad f(\mathbf{x}_0 \quad \varepsilon \mathbf{c}_i^T) \tag{22}$$

with the primal and dual parts given by

$$z_i \quad f(\mathbf{x}_0) \text{ and } \tilde{z}_i \quad \mathbf{c}_i \quad f(\mathbf{x}_0) \tag{23}$$

respectively. After n steps we obtain $\tilde{\mathbf{z}} \quad \mathbf{Cs}$ as the dual part of the auxiliary vector $\hat{\mathbf{z}}$. As the final step, we calculate

$$\hat{y} \quad f(\mathbf{x}_0 \quad \varepsilon \tilde{\mathbf{z}}) \tag{24}$$

in which the function value, $y(\mathbf{x}_0)$, is given by the real part of the result, and uncertainty is given by its dual part

$$y \quad f(\mathbf{x}_0) \text{ and } \mathrm{var}[y] \quad \tilde{y} \quad \mathbf{s}^T \tilde{\mathbf{z}} \tag{25}$$

This approach requires $(n + 1)$ evaluations of dual-function $f(\hat{\mathbf{x}})$ for the uncertainty propagation. It will be employed in our study, even though it is not the usual way of utilizing the sandwich formula.

APPLICATION TO THE MULTI-GROUP DIFFUSION EQUATION

When propagating uncertainties to a full core diffusion solution, two problems need to be solved. The first is the multi-group diffusion equation itself, and the second is the propagation of uncertainties to this solution.

In the special case of an infinite two-group reactor, the diffusion equation has an analytical solution. The two-group steady-state diffusion problem in an infinite medium can be formulated as

$$\begin{matrix} \Sigma_{a1} & \Sigma_{s1\to 2} \\ \Sigma_{s1\to 2} & \Sigma_{a2} \end{matrix} \begin{matrix} 0 & \phi_1 \\ 0 & \phi_2 \end{matrix} = \frac{1}{k_\infty} \begin{matrix} \nu\Sigma_{f1} & \nu\Sigma_{f2} \\ 0 & 0 \end{matrix} \begin{matrix} \phi_1 \\ \phi_2 \end{matrix} \tag{26}$$

In eq. (26), we assume no fission neutrons in the thermal group ($\chi_1 = 1$, $\chi_2 = 0$) and no up-scattering ($\Sigma_{s2\to 1} \quad 0$). Under these assumptions, the well-known analytical solution to this problem is [19, 20]

$$k_\infty \quad \frac{\nu\Sigma_{f1}}{\Sigma_{a1} \quad \Sigma_{s1\to 2}} \frac{\nu\Sigma_{f2} \quad \Sigma_{s1\to 2}}{\Sigma_{a2}(\Sigma_{a1} \quad \Sigma_{s1\to 2})}, \quad \phi_1 \quad \frac{\Sigma_{a2}}{\Sigma_{s1\to 2}}\phi_2 \tag{27}$$

Similarly, the solution of the adjoint problem can be obtained in a closed form

$$k_\infty^\dagger \quad k_\infty,$$
$$\phi_1^\dagger \quad \frac{1}{\Sigma_{a1} \quad \Sigma_{s1\to 2}} \frac{\nu\Sigma_{f1} \quad \Sigma_{a2}}{\nu\Sigma_{f2}} \quad \Sigma_{s1\to 2} \quad \phi_2^\dagger \tag{28}$$

Iterative numerical algorithms may be required in more complicated cases, such as problems with more than two energy groups, as discussed in [13].

We select the two-group diffusion problem, eq. (26), as our test problem and the multiplication factor, k_∞, as our response of interest. Our objective is, therefore, to propagate the uncertainties in the cross-section values to k_∞ for few-group diffusion calculations.

Three variants of uncertainty propagation will be explored, and will be discussed in the rest of this section in the following order:

- For the closed-form analytical solution of the problem, dual number arithmetic is used to evaluate both the function and the uncertainty in the solution.
- Solving the problem with the power iteration algorithm. The algebra of dual matrices is employed in this process.
- Solving the problem with the adjoint-weighted technique. Automatic differentiation is used to facilitate the calculation of the partial derivatives in the perturbation formula.

Equations (27) and (28) will be evaluated using conventional real number arithmetic to obtain reference values of the multiplication factor and the group-wise forward and adjoint fluxes.

Uncertainty propagation applied to the analytical formula

Since data for the capture and fission cross-sections are often provided separately, we make the substitution $\Sigma_{ag} \quad \Sigma_{cg} \quad \Sigma_{fg}$ (where $g = 1, 2$ are energy group indices) into eqs. (26)-(28). The analytical expression for k_∞ in eq. (27) can then be written as a function of a vector argument

$$f(\mathbf{x}) \quad \frac{x_5}{x_1 \quad x_3 \quad x_7} \frac{x_6 x_7}{(x_2 \quad x_4)(x_1 \quad x_3 \quad x_7)} \tag{29}$$

where the newly introduced independent variables x_i with $i = 1, 2, \ldots, 7$ represent the macroscopic cross-sections in the following order: x_1 – the fast capture, x_2 – the thermal capture, x_3 – the fast fission, x_4 – the thermal fission, x_5 – the fast neutron production, x_6 – the thermal neutron production, and x_7 – the fast removal. One may also observe that the function in eq. (29) is mildly non-linear. If uncertainty information is available for the input variables, the procedure described in the previous section may be applied directly to eq. (29) to calculate the uncertainty in the output quantities.

The power iteration method

For an arbitrary number of energy groups, G, the analytical solution of the diffusion problem may not be available, and one looks for a numerical solution of the eigenvalue problem. The power iteration method is a standard method used in nuclear reactor criticality calculations. Although its description may be found in the nuclear engineering textbooks (for instance, in [19-21]), we summarize it here for the sake of demonstrating its link with the algebra of dual matrices, as employed in our study. To this end, let us present the multi-group neutron diffusion equation in matrix form

$$\mathbf{M}\boldsymbol{\Phi} \quad \frac{1}{k}\mathbf{F}\boldsymbol{\Phi} \tag{30}$$

where the standard multi-group neutron diffusion notations are utilized: the flux $\boldsymbol{\Phi}$ vector contains group fluxes as its components; $\mathbf{M}$ – the migration and loss operator (in an infinite medium it reduces to a matrix $\mathbf{M}$ $_t$ $_s^T$, where Σ_t is a diagonal matrix containing group-wise total cross-sections and Σ_s – the scattering matrix), and $\mathbf{F}$ is the fission operator, defined as $\mathbf{F}$ $\boldsymbol{\chi}(\boldsymbol{\nu}$ $_f)^T$, where $\boldsymbol{\chi}$ and $\boldsymbol{\nu}\Sigma_f$ are column matrices containing the fission spectrum and group-wise nu-fission cross-sections, respectively. The adjoint problem is defined as

$$\mathbf{M}^\dagger\boldsymbol{\Phi}^\dagger \quad \frac{1}{k^\dagger}\mathbf{F}^\dagger\boldsymbol{\Phi}^\dagger \tag{31}$$

where for the problem considered in this study, $\mathbf{M}^\dagger$ = $= \mathbf{M}^T$. The multi-group diffusion equation in an infinite medium can be presented in the form of the *standard* eigenproblem of linear algebra. By introducing the so-called *fission source*, $\mathbf{v} = \mathbf{F}\boldsymbol{\Phi}$, one obtains the eigenvalue problem

$$\mathbf{A}\mathbf{v} \quad \lambda\mathbf{v} \tag{32}$$

where $\mathbf{A} = \mathbf{F}\mathbf{M}^{-1}$ and λ k. The adjoint problem can be presented in a similar way

$$\mathbf{A}^\dagger\mathbf{v}^\dagger \quad \lambda^\dagger\mathbf{v}^\dagger \tag{33}$$

where $\mathbf{A}^\dagger$ $\mathbf{F}^T(\mathbf{M}^{-1})^T$, see [20].

We assume that matrix $\mathbf{A}$ has a unique largest eigenvalue, λ_1, which means that $|\lambda_1|$ $|\lambda_2|$ $\cdots$ $|\lambda_G|$ 0. A numerical solution for the largest eigenvalue and a corresponding eigenvector, $\mathbf{v}_1$, can be found by using the power iteration, given in *Algorithm 1*, the numerical stability of which is enhanced by ensuring that vector $\mathbf{v}_1^{(\ell)}$ (where ℓ is the iteration index) is always of unit length [22]. Once the eigenvalue problems (32) and (33) are solved, the multi-group flux is calculated based on eqs. (30) and (31) as

$$\boldsymbol{\Phi} \quad \frac{1}{\lambda}\mathbf{M}^{-1}\mathbf{v}_1 \text{ and } \boldsymbol{\Phi}^\dagger \quad \frac{1}{\lambda_1^\dagger}(\mathbf{M}^{-1})^T\mathbf{v}_1^\dagger \tag{34}$$

respectively, where $\lambda_1^\dagger$ λ_1.

Algorithm 1. The enhanced power iteration [22]

Initialize $\mathbf{v}^{(0)}$ with an arbitrary vector such that $\left\|\mathbf{v}^{(0)}\right\|_2$ 1
for $k = 1,2, \ldots$ **do**
$\mathbf{w}$ $\mathbf{A}\mathbf{v}^{(\ell-1)}$
$\mathbf{v}^{(\ell)}$ $\mathbf{w}/\|\mathbf{w}\|_2$
$\lambda^{(\ell)}$ $[\mathbf{v}^{(\ell)}]^T\mathbf{A}\mathbf{v}^{(\ell)}$
end for

One can observe from eq. (34) and *Algorithm 1*, that the solution procedure involves dual matrix and scalar multiplications, additions (subtractions), and inversion of dual matrices, which can be calculated using eqs. (10) to (12).

The perturbation method

Another typical approach to sensitivity analysis is the Adjoint-Weighted Technique [23, 24]. In this approach, the uncertainty of the response is still calculated by the sandwich rule, eq. (20), and sensitivities are calculated by applying formulas from the perturbation theory. For instance, the sensitivity of the neutron multiplication factor, k, with respect to a cross-section, x_i, is given by

$$s_i \quad \frac{\partial k}{\partial x_i} \quad \frac{\left\langle \boldsymbol{\Phi}^\dagger \quad \frac{\partial \mathbf{M}}{\partial x_i} \quad \frac{1}{k}\frac{\partial \mathbf{F}}{\partial x_i} \quad \boldsymbol{\Phi} \right\rangle}{\left\langle \boldsymbol{\Phi}^\dagger \quad \frac{1}{k^2}\mathbf{F}\boldsymbol{\Phi} \right\rangle} \tag{35}$$

where the brackets indicate integration (summation) over space and energy. The partial derivatives in eq. (35) still have to be evaluated in some way. To this end, we again use the automatic differentiation based on dual number arithmetic. Therefore, if n stochastic variables are involved in the definition of migration and loss operator, $\mathbf{M}$, and fission operator, $\mathbf{F}$, these operators have to be evaluated for $i = 1, \ldots, n$ and that is achieved by applying eq. (15).

RESULTS AND DISCUSSION

This section describes the numerical example and analysis of the results.

Description of the numerical example

The three described approaches will be illustrated with a simple example problem, in this case, a pre-homogenized fuel assembly with cross-sections in two broad energy groups and reflective boundary conditions. Parameter values were taken from [16, 17], where relevant uncertainty data is also provided. The selection of this example can be supported by the following considerations. First, its local sensitivity analysis solution can be obtained analytically. Second, the uncertainty propagation problem has been solved in the aforementioned references by applying the global sensitivity analysis methods. It is of interest to compare results obtained in these works to those obtained in this study.

We group, as before in eq. (29), the relevant cross-sections into a vector in the order

$$\mathbf{x} \quad [\ c_1 \quad c_2 \quad f_1 \quad f_2 \quad \nu \quad f_1 \quad \nu \quad f_2 \quad s_{1\ 2}\ ]^T \tag{36}$$

The test problem depends, therefore, on seven stochastic quantities (inputs). Their mean values are

$$\mu \quad 10^{\ 2}$$
$$[0.5336 \ \ 2.693 \ \ 0.19124 \ \ 2.8438 \ \ 0.4920 \ \ 6.929 \ \ 2.063]^T \tag{37}$$

and the covariance matrix is

$$\mathbf{C} \quad 10^{\ 8} \begin{bmatrix} 0.4155 & 0.2168 & 0.0529 & 0.0237 & 0 & 0 & 0 \\ 0.2168 & 2.1383 & 0.0171 & 0.6447 & 0 & 0 & 0 \\ 0.0529 & 0.0171 & 0.0170 & 0.0132 & 0 & 0 & 0 \\ 0.0237 & 0.6447 & 0.0132 & 0.8437 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.2311 & 0.1791 & 0 \\ 0 & 0 & 0 & 0 & 0.1791 & 9.6360 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 5.2816 \end{bmatrix} \tag{38}$$

In eqs. (37) and (38) cross-sections are given in cm^{-1} and the variances are given in cm^{-2}.

Analysis

The analytical solution of the considered diffusion problem, eqs. (27) and (28), was calculated with real number arithmetic and reference values were obtained for the multiplication factor, as well as the normalized forward and adjoint fluxes

$$k_\infty \quad k_\infty^\dagger \quad 1.10255$$
$$\mathbf{\Phi} \quad [1.0, 0.37260] \text{ and } \mathbf{\Phi}^\dagger \quad [0.88102, 1.0] \tag{39}$$

These values were then used to verify the solutions obtained in the first two applications (namely, analytical dual function evaluation and dual power iteration solution), as well as in the perturbation formula, eq. (35).

Dual number calculations for the diffusion solution, as well as uncertainty propagation based on dual number automatic differentiation, were implemented in the high-level, high-performance, dynamic programming language Julia [25]. For dual number algebra, we used the DualNumbers Julia module, and for dual matrix operations, we employed the DualMatrixTools Julia module [26]. The analytical solution with dual number arithmetic and the dual algebra power iteration solution both produce the same values for k_∞, $\mathbf{\Phi}$ and $\mathbf{\Phi}^\dagger$, to within working precision ($2\ 10^{-16}$), as compared to the reference.

All three approaches yield the same result for the uncertainty up to the 6th significant figure, and the results are summarized in the first three rows of the tab. 1. The uncertainty is reported in two ways. Firstly, for the sake of comparison with results from the literature, in terms of the standard deviation of the multiplication factor, $\sigma_k \quad \sqrt{\mathrm{var}[k]}$. The second way is in terms of percentage relative standard deviation, 100 % $\delta k/k$ (where δk stands for σ_k), as is customary in the field.

The calculated uncertainty values are compared with values from [16, 17], where the test problem under consideration was initially introduced. Results in these references were obtained by various global sensitivity analysis methods, including Monte Carlo sampling, quasi Monte Carlo and sparse grid quadratures, as well as the asymptotic approximation. In addition, two of the global sensitivity analysis methods, namely Monte Carlo sampling and sparse grid quadrature, were reimplemented in this study to more accurately determine the number of samples (*i. e.* diffusion solutions) that are required to obtain a given precision of results. The uncertainty calculated with the various global sensitivity analysis methods is also reported in tab. 1.

Inspection of results in the table reveals that all the methods yield uncertainty values that are close to each other. It is particularly interesting to observe the similarity between results from local and global approaches, which indirectly supports the rationale of the asymptotic approximation in [17]. This approach assumes that for small input uncertainties, the uncertainty of the response is given by the linearised part of

Table 1. Uncertainty and the required number of diffusion calculations for different methods as applied to the two-group test problem

Method	Number of samples	Uncertainty	
		$_k\ 10^{-3}$	$\delta k/k$ [%]
Automatic differentiation (local sensitivity analysis method)			
Analytical formula	7*	5.9796	0.5423
Power iteration	7*	5.9796	0.5423
Perturbation formula	2	5.9796	0.5423
Global sensitivity analysis methods (this work)			
Gauss-Hermite sparse grid quadrature	15	5.9796	0.5423
Monte Carlo sampling/quadrature	10^7	5.9806	0.5423
Global sensitivity analysis methods (from literature)			
Monte Carlo sampling/quadrature [16]	10^5-10^6	5.979	0.5423
Randomized quasi Monte Carlo quadrature [16]	10^4-10^5	5.980	0.5424
Gauss-Patterson sparse grid quadrature [16]	29	5.972	0.5417
Asymptotic approximation [17]	7	5.979	0.5423

*Requires evaluation of dual number-valued functions

the model. As far as our test problem is concerned, these results indicate that the local sensitivity analysis procedure based on the automatic differentiation and sandwich rule provides an accurate estimation of the output uncertainty.

The computational cost is, however, different for different methods. One may observe in tab. 1 that, for the problem under consideration, the automatic differentiation technique requires the smallest number of samples, followed by the sparse grid quadrature, while the Monte Carlo methods require several orders of magnitude more samples. When performing this comparison, several factors have to be taken into account.

Firstly, dual-function evaluations require a small factor with more arithmetic operations than the original real number evaluation (the factor varies from two for addition and subtraction to six for division). Tables with the factors for different operations can be found, *e. g.* in [9, 10].

Secondly, the methods under consideration scale differently for bigger problems. In this problem, there are seven uncertain input parameters. We show, as an example, an approach in which eight dual function evaluations are used, though the number of function evaluations can be reduced to seven by calculating the gradient directly, at the additional cost of the sandwich formula evaluation. More generally, the first two approaches require n or $n + 1$ dual function evaluations, where n is the number of uncertain input parameters. The perturbation formula requires n dual evaluations of operators involved in the diffusion equation, while, the diffusion problem has to be solved only twice: the forward problem to obtain $\mathbf{\Phi}$ and the adjoint problem to obtain $\mathbf{\Phi}^\dagger$.

Furthermore, based on the results of this study, and the properties of sparse grids, we expect that the number of required samples is, at least, $(2n + 1)$ for sparse grid-based methods. One may also observe that Gauss-Hermite sparse grid quadrature, employed in our study, required a smaller number of samples than its Gauss-Patterson counterpart. This difference may be attributed to the quadrature weight used. The Gauss -Hermite quadrature includes e $^{\|\mathbf{x}^2\|}$ as weight, which may be the reason for its improved efficiency.

Our next comment is about the asymptotic approximation method, which in practice reduces to the sandwich formula. This means the components of the sensitivity vector must be calculated in some way. In [17], sensitivities were calculated analytically for the asymptotic approximation. If automatic differentiation is employed to do so, the same number of dual-function evaluations would be required as for the analytical or power iteration approaches, *i. e.*, n or $n + 1$.

Finally, unlike previously discussed approaches, Monte Carlo methods are known to converge as the square root of the number of samples, regardless of the number of input variables. It may, therefore, become comparatively more computationally efficient for particularly large problems.

CONCLUSIONS

In this study, we consider the problem of propagating uncertainty from group-wise neutron cross-sections to the results of neutronics diffusion calculations. We employed automatic differentiation in conjunction with the sandwich formula for uncertainty propagation in three different ways. Firstly, by evaluating the analytical expression for the multiplication factor using dual number arithmetic. Then, by solving the diffusion problem with the power iteration algorithm and the algebra of dual matrices. Finally, automatic differentiation is used to facilitate the calculation of partial derivatives of the production and loss operators in the perturbation formula in the context of the adjoint-weighted technique.

The solution to the two-group diffusion equation as calculated using dual number arithmetic recovered the reference solution obtained with conventional real numbers exactly. This holds for both the analytic formula and the power iteration method. All three uncertainty propagation methods applied in this work yielded the same result for the uncertainty of the multiplication factor. Furthermore, they showed excellent agreement with the global methods used for comparison, with differences below $1\ 10^{-5}$ in all cases.

Uncertainty propagation and sensitivity analysis based on automatic differentiation can be seen as a useful addition to the traditionally used sampling or perturbation methods, especially due to the possible savings in computational cost associated with it.

AUTHORS' CONTRIBUTIONS

P. M. Bokov proposed the research concept and methodology, as well as performed the formal analysis. All the authors contributed to writing the original draft and to the preparation of the final version of the manuscript.

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ПРИМЕНА АУТОМАТСКОГ ДИФЕРЕНЦИРАЊА ЗАСНОВАНОГ НА АРИТМЕТИЦИ ДУАЛНИХ БРОЈЕВА НА ПРОПАГАЦИЈУ НЕОДРЕЂЕНОСТИ ДВОГРУПНИХ НЕУТРОНСКИХ ПРЕСЕКА

Тема овог рада је проблем пропагације неодређености групних неутронских пресека у глобалним дифузионим прорачунима нуклеарних реактора. Аутоматско диференцирање засновано на аритметици дуалних бројева је примењено на пропагацију неодређености у оквиру анализе локалне осетљивости. Као илустрација, размотрен је двогрупни критични дифузиони проблем у бесконачној средини, који има аналитичко решење. Аутоматско диференцирање у комбинацији са сендвич формулом за пропагацију неодређености примењено је на три различита начина. Прво је фактор мултипликације израчунат аналитички применом аритметике дуалних бројева. Затим је критични дифузиони проблем решен методом итерације фисионог извора и применом алгебре дуалних матрица. Коначно, парцијални изводи оператора производње и губитака у пертурбационој формули са адјунгованом тежинском функцијом израчунати су помоћу аутоматског диференцирања. Нумеричко решење дифузионог проблема је верификовано упоредјивањем са аналитичким решењем. Резултати прорачуна неодређености упоређени су са резултатима добијеним применом методе глобалне анализе осетљивости. Вредности неодређености израчунате у овом раду слажу се унутар $1 \cdot 10^{-5}$ са вредностима датим у литератури.

Кључне речи: аутоматско диференцирање, дуални бројеви, сендвич формула, анализа осетљивости, пропагација неодређености, итерација фисионог извора