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ANOVA DERIVATIVE-BASED SENSITIVITY WITH APPLICATIONS TO A PLASMA–COMBUSTION SYSTEM

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Abstract. We review and analyze derivative-based sensitivity measures, and propose efficient numerical approach to estimate these measures. These measures are then applied to combustion and plasma problems. Non-important parameters are successfully identified and neglected for more complex applications.

1 INTRODUCTION

Kucherenko et al. [1], Sobol' and Kucherenko [2, 3] introduced derivative-based sensitivity indices (DSI) and have shown a link with the variance-based total sensitivity indices (Var-TSI). Even though Var-TSI are considered superior to DSI for importance ranking because they contain more model information (e.g. higher-order and mixed derivatives), their cost is higher [1–3], which can restrict their use. For example, Monte Carlo (MC) algorithms for DSI and Var-TSI have been developed and compared, and DSI convergence can be much faster than Var-TSI, particularly in applications with little derivative variation. The approach proposed by Sudret and Mai [4] aims to estimate the DSI [2] based on a polynomial chaos expansion. However, the extension of this for other DSI [3] seems difficult because the additional terms in the integrand disrupt orthogonality. In following, we review and analyze derivative-based measures for inputs of arbitrary probability distribution and show how they can be estimated using an efficient adaptive Analysis of Variance (ANOVA) surrogate [5, 6]. We then use them in combustion and laser-induced breakdown applications, with 18 and 16 uncertain parameters, respectively.

2 DERIVATIVE-BASED SENSITIVITY INDICES (DSI)

2.1 Basic definitions of DSI

The original derivative-based sensitivity indices (DSI) proposed by Kucherenko et al. [1] for a quantity of interest $f(\vec{x})$, depending on uncertain parameters $\vec{x}$, measure the average of the gradient sensitivity over the input space,

$$\mu_i = \int_{\mathbb{R}^N} \frac{\partial f(\vec{x})}{\partial x_i} \, \mathrm{d}F_{\vec{x}}(\vec{x}), \tag{1}$$

where $F_{\vec{x}}(\vec{x})$ is the joint cumulative distribution function of $\vec{x}$. A drawback of this Morris-like measure is that the integrand in (1) can be positive and negative, which may lead to underestimate of the parameter's relative importance. Campolongo et al. [7] thus proposed to use the approximated values of $|\frac{\partial f}{\partial x_i}|$ within the framework of the Morris method [8]. In this spirit, Kucherenko et al. [1] redefined

$$\mu_i^* = \int_{\mathbb{R}^N} \left| \frac{\partial f(\vec{x})}{\partial x_i} \right| \, \mathrm{d}F_{\vec{x}}(\vec{x}). \tag{2}$$

It is established that the Monte Carlo or Quasi Monte Carlo integration method proposed by Kucherenko et al. [1] for DSI is more efficient and accurate than the original Morris method. It has also been argued that the cost for numerical evaluation of DSI is many orders of magnitude lower than that of Sobol' variance-based total sensitivity indices (Var-TSI) $\mathcal{S}_{i,\mathbf{T}}$ [1].

It has been noticed on particular cases that the measure μ_i^* gives a similar parameter ranking as Var-TSI. However, no proof links μ_i^* and Var-TSI. To establish a link, Sobol' and Kucherenko [2] proposed the following DSI

$$\nu_i = \int_{\mathbb{R}^N} \left(\frac{\partial f(\vec{x})}{\partial x_i} \right)^2 \, \mathrm{d}F_{\vec{x}}(\vec{x}), \tag{3}$$

and show, in the case of uniformly distributed $\vec{x} \in [0,1]^N$, that

$$\mathcal{S}_{i,\mathbf{T}} \leq \frac{1}{\pi^2} \frac{\nu_i}{V}, \tag{4}$$

with $V = \int_{\mathbb{R}^N} (f - E(f))^2 \, \mathrm{d}F_{\vec{x}}(\vec{x})$ the total output variance. The importance of (4) is that small $\frac{\nu_i}{V}$ implies small $\mathcal{S}_{i,\mathbf{T}}$, so unimportant parameters can be neglected based on relative ν_i.

Using the first-order approximation of the Taylor expansion of Var-TSI, Sobol' and Kucherenko [3] further proposed a new DSI:

$$\tau_i = \frac{1}{2} \int_{\mathbb{R}} \int_{\mathbb{R}^N} \left(\frac{\partial f(\vec{x})}{\partial x_i} \right)^2 (x_i - x_i')^2 \, \mathrm{d}F_{\vec{x}}(\vec{x}) \, \mathrm{d}F_i(x_i'). \tag{5}$$

It can be impractical to compute (5) for a general random vector $\vec{x}$, since $\vec{x}$ and x_i' need to be independently sampled. However, we recognize

$$(x_i - x_i')^2 = (x_i - E_i)^2 + (x_i' - E_i)^2 - 2(x_i - E_i)(x_i' - E_i), \tag{6}$$

where $E_i = \int_{\mathbb{R}} x_i \, \mathrm{d}F_i(x_i)$. The last term in (6) does not contribute to the integral (5). If we further define a sensitivity measure ζ_i as

$$\zeta_i = \int_{\mathbb{R}^N} \left(\frac{\partial f(\vec{x})}{\partial x_i} (x_i - E_i) \right)^2 \mathrm{d}F_{\vec{x}}(\vec{x}), \tag{7}$$

τ_i in (5) can be expressed

$$\tau_i = \frac{1}{2}(\zeta_i + V_i \nu_i), \tag{8}$$

with $V_i = \int_{\mathbb{R}} (x_i - E_i)^2 \, \mathrm{d}F_i(x_i)$ the variance of input parameter x_i. It should be noted that (8) does not provide any restriction to the distribution for random variables $\vec{x}$; particularly, it does not need to be uniform or normal. For linear problems, we immediately have

$$\mathcal{S}_{i,\mathbf{T}} = \frac{V_i \nu_i}{V} = \frac{\tau_i}{V} = \frac{\zeta_i}{V}. \tag{9}$$

Thus, $V_i \nu_i$, τ_i and ζ_i are good approximations of Var-TSI. We will assess these three derivative-based measures in application examples.

We thus estimate τ_i by using (8) and a combination of standard Monte Carlo algorithm with an adaptive ANOVA surrogate constructed with significantly fewer samples [5, 6, 9].

2.2 Uniformly distributed random variables

To further explain the link between Var-TSI and the three DSI measures ν_i, τ_i, and ζ_i, we follow Sobol' and Kucherenko [3] and consider uniformly distributed random variables $\vec{x} \in [0,1]^N$. Sobol' and Kucherenko [3] proposed and analyzed

$$\tau_i^{(1)} = \int_{\mathbb{R}^N} \left(\frac{\partial f(\vec{x})}{\partial x_i} \right)^2 \frac{1 - 3x_i + 3x_i^2}{6} \, \mathrm{d}\vec{x}. \tag{10}$$

Since $1 - 3x_i + 3x_i^2$ is bounded for $x_i \in [0,1]$, we have

$$\frac{1}{24}\nu_i \leq \tau_i^{(1)} \leq \frac{1}{6}\nu_i. \tag{11}$$

Considering (4) and (11), Sobol' and Kucherenko [3] have concluded

$$\mathcal{S}_{i,\mathbf{T}} \leq \frac{1}{\pi^2}\frac{\nu_i}{V} \leq \frac{24}{\pi^2}\frac{\tau_i^{(1)}}{V}. \tag{12}$$

Thus, small $\frac{\tau_i^{(1)}}{V}$ also implies small Var-TSI.

We can similarly express (7) as

$$\zeta_i^{(1)} = \int_{\mathbb{R}^N} \left(\frac{\partial f(\vec{x})}{\partial x_i} \right)^2 \frac{1 - 4x_i + 4x_i^2}{4} \, \mathrm{d}\vec{x}. \tag{13}$$

It should be clear that

$$0 \leq \zeta_i^{(1)} \leq \frac{1}{4}\nu_i, \tag{14}$$

so a small ν_i implies a small $\zeta_i^{(1)}$. However, such a a theoretical link does not exist between Var-TSI $\mathcal{S}_{i,\mathbf{T}}$ and $\zeta_i^{(1)}$.

2.3 Comparison of Monte Carlo algorithms

Though the proposed approach does not rely on uniformly distributed random variables, we can make firm estimates of cost and accuracy for this special case. By considering a model with a linear dependence with respect to x_i, Sobol' and Kucherenko [3] compared the costs of Monte Carlo algorithms for computing τ_i (5), $\tau_i^{(1)}$ (10) and ν_i (3). Let N_1, N_2 and N_3 be respectively the numbers of the sample sizes required to achieve a given relative error. Sobol' and Kucherenko [3] showed that

$$2 < \frac{N_1}{N_2} \leq 7, \qquad \frac{12}{5} < \frac{N_1}{N_3} \leq \infty. \tag{15}$$

Denote by N_4 the sample size required to obtain the same relative error for $\zeta_i^{(1)}$ (13). We can similarly assert

$$\frac{4}{3} < \frac{N_1}{N_4} \leq \frac{7}{4}. \tag{16}$$

From (15) and (16), the sample size for τ_i must be larger than for $\zeta_i^{(1)}$, and several times larger than for $\tau_i^{(1)}$ and ν_i. The convergence rate of $\zeta_i^{(1)}$ seems inferior than $\tau_i^{(1)}$ for the linear case. However, in a nonlinear case, Sobol' and Kucherenko [3] have shown models for which we have $\frac{N_1}{N_2} < 1$. In practice, we have not noticed a significant difference in terms of convergence between $\zeta_i^{(1)}$ and $\tau_i^{(1)}$.

3 SURROGATE-BASED ESTIMATION OF DSI

The purpose of this work is to propose an efficient methodology to compute DSI (3) and (5) for any type of random variables (not restricted to uniform or normal variables). While it is always possible to estimate these integrals by crude Monte Carlo to obtain realizations of computer simulations, this approach is however prohibitive in many challenging cases due to computational cost, such as for the plasma-combustion systems we consider here [6].

Using a polynomial surrogate to replace the original simulation model is an efficient method, especially when the output statistics and sensitivity indices can be obtained by manipulating polynomial coefficients. The analytical derivatives for a given system of orthogonal polynomials are known to be linear combinations of at most two polynomials of the same system [10]. Sudret and Mai [4] used the analytical derivatives to compute ν_i (3) by taking advantage of the orthogonality of classical polynomials. Computing ν_i is very similar to the variance computation using a Polynomial Chaos expansion. However, this approach can be inconvenient for DSI containing additional terms in the integrand, particularly because its advantageous properties due to orthogonality are lost.

As an alternative, a simple approach of computing (3), (5), and (7) is by standard Monte Carlo sampling of an accurate surrogate. The derivative $\frac{\partial f(\vec{x})}{\partial x_i}$ can still be obtained analytically from the surrogate representation. The challenge becomes the construction of meta-models from a relatively small number of full model evaluations. For this, we use a recently proposed adaptive ANOVA method [5, 6].

4 APPLICATION EXAMPLES

There are many and varied uncertainties in the plasma-coupled combustion systems [6, 11], so we consider dimension reduction based on lower-dimensional (less involved and less expensive) configurations exposing similar physical phenomena [6]. We consider two low-dimensional models featuring multiphysics parameters here, both of which can be used for this purpose.

4.1 Premixed flame speed — A quasi-linear case

We consider the laminar propagation velocity of hydrogen–air planar deflagrations with initial temperature $T_u = 300\,\mathrm{K}$ and pressure $P = 1\,\mathrm{atm}$. The San Diego mechanism [12] is used, which has 20 reversible elementary reactions among eight species, $H_2, O_2, H_2O, H, O, OH, HO_2, H_2O_2$. It is known that the uncertainties of transport coefficients are as important as those of chemical-kinetic rate parameters, especially for hydrogen combustion due to high diffusivity of light species H_2, H [12–14]. Combustion reactions are generally strongly nonlinear, and we will study them in a future work [15]. We thus only focus on transport properties as sources of uncertainty in this example.

The transport models we use are standard [16–18]. An intermolecular potential model is needed to evaluate the collision integrals that provide transport coefficients. Following Kee et al. [16], we use the widely employed Lennard–Jones 12–6 potential model,

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right],$$

where ϵ is the depth of the potential well (the maximum attractive energy), and σ the nominal collision cross-section for low-energy collisions (the distance at which the potential is zero). The uncertainties of ϵ and σ for the eight reactive species and N_2 are reported in Table 1. We assume a uniform distribution for these parameters, and the min/max are

Species	$\epsilon_{\min}/k$ (K)	$\epsilon_{\max}/k$ (K)	$\sigma_{\min}$ ($\times 10^{-10}$ m)	$\sigma_{\max}$ ($\times 10^{-10}$ m)
H_2	33.300	59.700	2.827	2.968
H	37.000	145.000	2.050	2.708
O_2	106.700	121.100	3.407	3.467
O	80.000	106.700	2.750	3.050
OH	79.800	809.100	2.605	3.147
HO_2	107.400	365.560	3.433	4.196
H_2O_2	107.400	368.110	3.460	4.196
H_2O	535.210	809.100	2.600	2.673
N_2	71.400	98.400	3.620	3.798

Table 1: Transport coefficients uncertainties. k is the Boltzmann constant.

taken from previously reported literature [14, 19, 20].

Figure 1 shows the mean and standard deviation of laminar flame velocity of hydrogen-

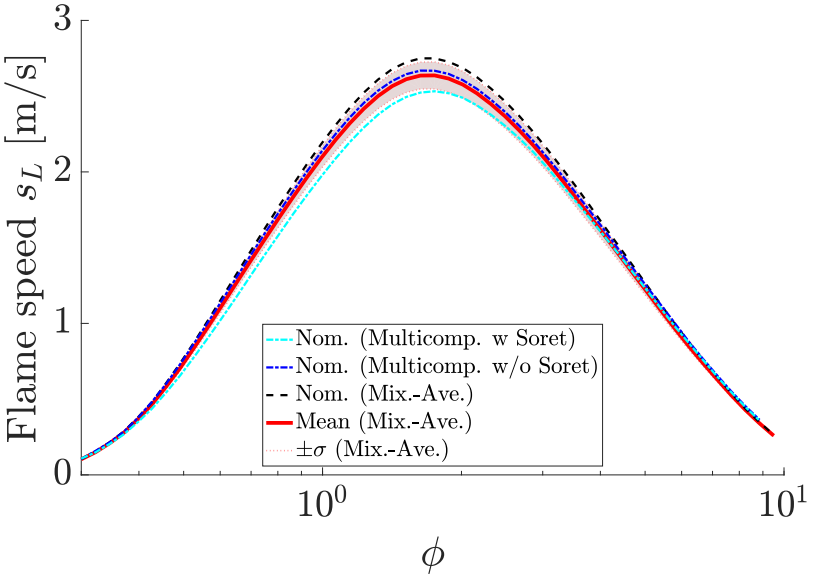

Figure 1: The variation of flame speed s_L with respect to the equivalence ratio ϕ, and the uncertainty of s_L due to transport properties.

air planar deflagrations due to uncertainties of mixture-averaged transport model (Table 1), compared to the flame speed obtained using nominal coefficients (codes of Kee et al. [16, 17] incorporated in CHEMKIN[1]) in both mixture-averaged and multi-component transport models. The output uncertainty of s_L seems small. However, when the flame is stretched or curved in a three-dimensional diffusion flame, uncertainty can be significant in particular for hydrogen combustion [12]. Thus, the sensitivity analysis of transport properties is deemed necessary to identify the influential transport parameters. Figure 2 shows the sensitivity indices. Figure 2a compares three DSI: $V_i\nu_i = \frac{1}{12}\nu_i$ (3), ζ_i (7), and τ_i (5) or (8). We observe that these three measures consistently indicate the significance of the H radical. The importance of the H radical can be anticipated because of its central contribution to $H + O_2 \rightleftharpoons OH + O$, which is known to be an important elementary reaction for the description of hydrogen combustion. Its reaction rate (depending partly on H concentration) influences fundamentally any hydrogen-containing combustion [12]. We further plot the input–output dependence in Figure 3, where a quasi-linear dependence can be observed between s_L and σ. This quasi-linear relationship can also be inferred based on the three very close index values of σ_H shown in Figure 2a. In fact, these three DSI should be equal for a linear problem (9). Figure 2b presents the variance-based total sensitivity indices (Var-TSI) [6], which provides identical importance information as DSI, and further increases our overall confidence.

[1]A chemical kinetics software tool: http://www.reactiondesign.com/products/chemkin

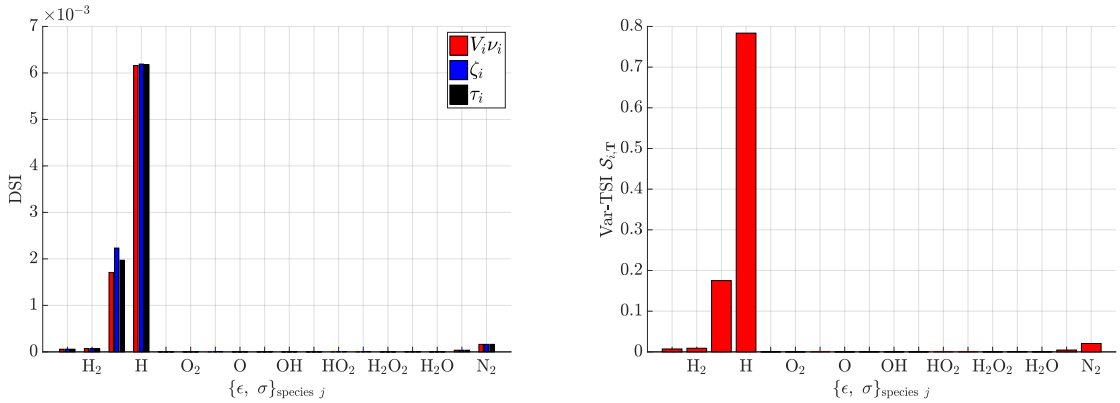

Figure 2: Sensitivity analysis of laminar flame speed on transport coefficients: (a) derivative-based sensitivity indices (DSI); (b) variance-based total sensitivity indices (Var-TSI).

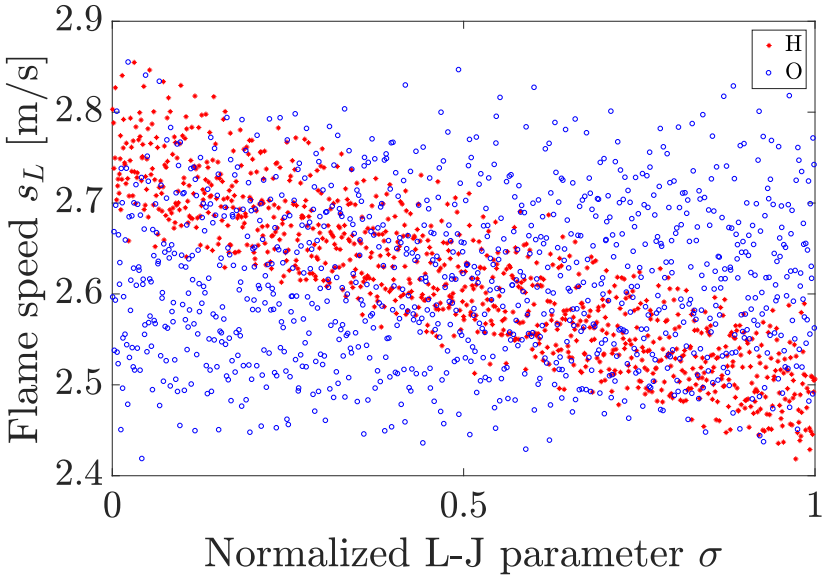

Figure 3: Flame speed s_L vs. the collision diameter σ of H, O.

4.2 Laser-induced breakdown (LIB) — A non-monotone case

Munafò et al. [21] discussed the modeling of laser-induced breakdown (LIB) in gases, which has been used as an ignition seed for supersonic plasma-coupled combustion [15]. This LIB model couples fluid motion of non-equilibrium material gas with a radiation field, and contains a large number of uncertain parameters. Uncertainty quantification of this LIB model in full-scale is challenging, not only because there is a large range of time-scales (from pico- to nano-seconds for ionization and breakdown, and up to micro-

seconds for hydrodynamics), but it also must account for the most important collisional and radiative processes. Because of all above difficulties, it is preferable for us to first neglect non-influential parameters by realizing a sensitivity study of the LIB model with a zero-dimensional configuration. We do keep in mind that dimension-related phenomena cannot be taken into account in this uncertainty analysis, for example transport properties.

The initial pressure and temperature correspond to the conditions at the outlet of the nozzle of the ACT-II facility at the University of Illinois. Based on the experiments, we consider a LIB in a gas mixture of H_2, O_2. The underlying kinetics can be modeled as a reaction scheme (17):

$$
\begin{array}{lllll}
(1) & \mathrm{O_2 + M} & \rightleftharpoons & \mathrm{O + O + M}, & \mathrm{M = O\,,\quad O^+} \\
(2) & \mathrm{O_2 + M} & \rightleftharpoons & \mathrm{O + O + M}, & \mathrm{M = O_2\,,\quad {O_2}^+} \\
(3) & \mathrm{O + e^-} & \rightleftharpoons & \mathrm{O^+ + e^- + e^-} & \\
(4) & \mathrm{O^+ + e^-} & \rightleftharpoons & \mathrm{O^{2+} + e^- + e^-} & \\
(5) & \mathrm{O_2 + e^-} & \rightleftharpoons & \mathrm{{O_2}^+ + e^- + e^-} & \\
(6) & \mathrm{O + O} & \rightleftharpoons & \mathrm{{O_2}^+ + e^-} & \\
(7) & \mathrm{O + {O_2}^+} & \rightleftharpoons & \mathrm{O_2 + O^+} & \\
(8) & \mathrm{H_2 + M} & \rightleftharpoons & \mathrm{H + H + M}, & \mathrm{M = H\,,\quad H^+} \\
(9) & \mathrm{H_2 + M} & \rightleftharpoons & \mathrm{H + H + M}, & \mathrm{M = H_2} \\
(10) & \mathrm{H + e^-} & \rightleftharpoons & \mathrm{H^+ + e^- + e^-} & \\
(11) & \mathrm{H_2 + e^-} & \rightleftharpoons & \mathrm{{H_2}^+ + e^- + e^-} &
\end{array}
\tag{17}
$$

Munafò et al. [21] provide estimated rate parameters. The pre-exponential factors $\{A_k\}$ in the Arrhenius equation are known to be the main sources of uncertainty in reaction models. We thus consider a log-uniform distribution for the pre-exponential $\{A_k\}$:

$$\log_{10} A_k \pm 1, \qquad k = 1, \cdots, 11.$$

Other uncertain parameters of the LIB considered in this work include the absorption cross-section $\mathcal{Q}$, the free-electron mole fraction $X_{e,0}$, the focal radius r_f, the input laser energy E_{laser}, and the Full Width at Half Maximum (FWHM) of the laser pulse. Readers are referred to Munafò et al. [21] for the role of these parameters in LIB. The values and uncertain ranges of these parameters correspond to experiments [15, 21], and are reported in (18).

$$
\begin{array}{lcll}
\mathcal{Q} & \sim & \mathcal{U}(1. \times 10^{-13}, \quad 1. \times 10^{-12}) & [\mathrm{m^2\,K}] \\
X_{e,0} & \sim & \mathcal{U}(1. \times 10^{-9}, \quad 1. \times 10^{-8}) & [\text{-}] \\
r_f & \sim & \mathcal{U}(50. \times 10^{-6}, \quad 150. \times 10^{-6}) & [\mathrm{m}] \\
E_{\text{laser}} & \sim & \mathcal{U}(300 - \frac{300}{100}, \quad 300 + \frac{300}{100}) & [\mathrm{m\,J}] \\
\mathrm{FWHM} & \sim & \mathcal{U}(8.^{-9} - \frac{8.^{-9}}{100}, \quad 8.^{-9} + \frac{8.^{-9}}{100}) & [\mathrm{s}]
\end{array}
\tag{18}
$$

The model output of interest is the post-breakdown temperature T. The Morris-like DSI μ_i and μ_i^* are shown in Figure 4. The difference in magnitudes of μ_i and μ_i^* implies that the model output depends non-monotonically on input parameters. We do have

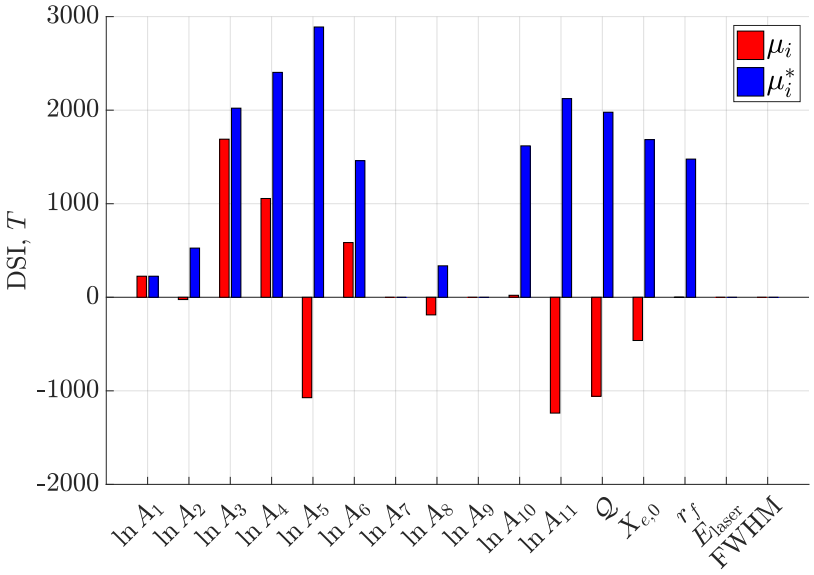

Figure 4: Morris-like DSI μ_i and μ_i^* for LIB model.

relatively small μ_i and μ_i^* values for several parameters. However, it is unclear whether it is safe to neglect $A_{1,2,8}$. Three other DSI $V_i\nu_i$, ζ_i and τ_i are then reported in Figure 5. Unlike the simpler flame speed case in Section 4.1, we now have very different values of

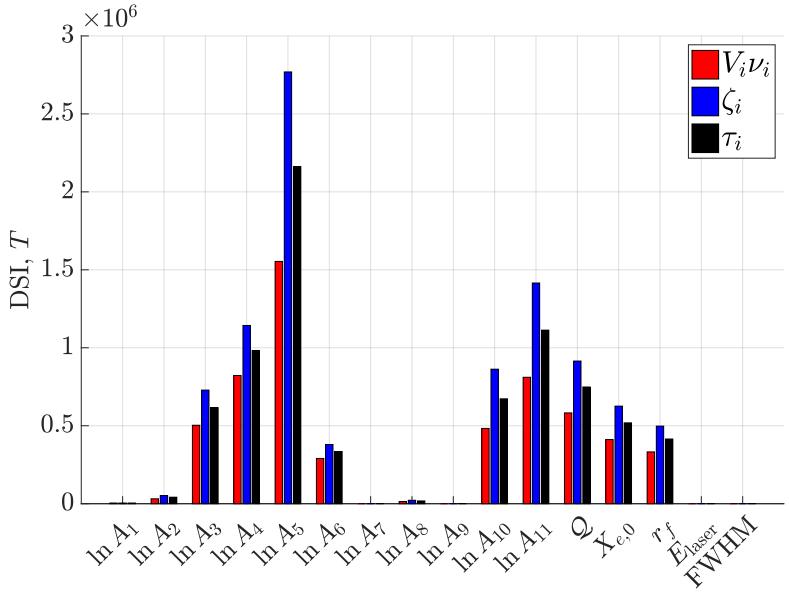

Figure 5: DSI $V_i\nu_i$, ζ_i and τ_i for LIB model.

these three DSI for each parameter, because of the non-monotonic input–output relation. However, the relatively small DSI values of $A_{1,2,7,8,9}$, E_{laser} and FWHM guarantee their small Sobol' total sensitivity indices (Var-TSI) per (12). We thus can confidently neglect

these 7 parameters. The remaining 9 parameters would be retained for subsequent stages of the overall UQ effort.

5 CONCLUSIONS

We have reviewed existing definitions of derivative-based sensitivity indices (DSI), including the Morris-like measures (1) and (2), and more recently ν_i (3) by Sobol' and Kucherenko [2] and τ_i (5) by the same authors [3]. These measures are all functionals depending on $\frac{\partial f}{\partial x_i}$ which have been suggested as importance estimators of parameter x_i. Generally speaking, DSI are less expensive to compute than variance-based total sensitivity indices (Var-TSI) by Monte Carlo approaches [1–3], so they are attractive tools for dimension reduction when the system of interest has a large number of uncertain parameters.

We then propose an approach (8) to compute τ_i (5) using a combination of ν_i (3), ζ_i (7) and the input variance V_i. Uncertain parameters are not restricted to be random variables in the Polynomial Chaos Askey scheme. The novelty of this approach is to use an adaptive sparse polynomial surrogate for the sampling procedure. Even though the cost of computing Var-TSI is significantly lower using the adaptive approach [5, 6] than Monte Carlo, it still requires, for complex problems, to build highly accurate meta-models by using high-degree polynomials in order to estimate high-order and mixed derivatives in the Var-TSI formulation. Such a high precision is not necessary to compute DSI, since DSI only contain first-order derivatives and are specifically designed as screening methods to disregard unimportant parameters. In this sense, DSI are still less expensive in practice than Var-TSI even when using a surrogate approach.

An example of laminar flame speed with uncertain transport properties has been studied, which represents a practical case where the input–output relationship is quasi-linear. Thus, one expects that the DSI $V_i\nu_i$, ζ_i and τ_i provide identical importance ranking as the variance-based global sensitivity indices [3]. A second example of laser-induced breakdown in plasma was also studied. Uncertain parameters include kinetics rate parameters and other laser or radiation model parameters. The input–output relation is non-monotonic in this second case, and we have concluded that DSI based on $(\frac{\partial f}{\partial x_i})^2$ can be more helpful than Morris-like indices μ_i and μ_i^*.

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