Uncertainty analysis approximation for non-linear processes using Telemac-AD

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***Abstract*—The first-order second-moment (FOSM) is an uncertainty analysis method that assumes a first-order Taylor series expansion at the central value of the input variables to estimate the output variance. The expansion at central values with a first-order approximation might introduce large over- or underestimation when dealing with non-linearities. If the variance assumed for the input parameters is not small enough, the assumption of linearity or slightly non-linearity in this method might be violated.**

In FOSM the variance of the output variables is approximated by the product of the variance of the input parameters and the partial derivative of the model variable with respect to each parameter. In this study we propose to substitute the Gaussian distribution of a model input parameter with high variance by several Gaussian distributions with smaller variances. The weighted combination of the multiple distributions (Compound FOSM or CFOSM) represents nearly the same distribution as the original one (FOSM). In CFOSM the uncertainty analysis has to be carried out for each member of the compound distribution. For this reason the computing time is increased by the number of members considered. Yet, non-linearities can be better approximated and the new approach still requires much less computing time than the Monte Carlo method.

Uncertainty analysis based on the proposed approach will be carried out with validation test cases from the Telemac-Mascaret System. The partial derivatives will be calculated by means of Algorithmic Differentiation efficiently. Results from the analysis of each test case with FOSM and CFOSM will be compared to a Monte Carlo Simulation.

I. INTRODUCTION

Uncertainty analysis attempts to describe the entire set of possible outcomes of an event, together with their associated probabilities of occurrence. It can be very helpful to identify input parameters that produce the largest uncertainties in hydro- and morphodynamic modeling. Since the 1980's this technique has been employed to hydraulic and hydrological modeling ([1],[2],[8]) usually associated to structure and risk analysis in engineering. Since then the method is still found in use and its application has been extended also to sediment transport and morphodynamic modeling ([6],[7],[9],[10],[15]).

Especially in morphodynamic modeling the sensitivity analysis of relevant parameters and, finally, the determination of their uncertainty contribution on end results should be addressed. This recommendation is simply based on the mathematical formulations of sediment transport (e.g. initiation of motion, bedload). These are essentially empirical and might lead to significant errors depending on the time scale considered.

In this manuscript uncertainty analysis will be carried out by applying the first-order second-moment (FOSM) method. Hydrodynamic and morphodynamic processes are described by non-linear relations. However, the direct application of the FOSM method using a typical variation range for the input parameters, e.g. according to measurement uncertainties, could lead to excessive large variances. The main goal here is to properly address non-linearities by means of a new approach based on the FOSM. In order to test the proposed method, two test cases from Telemac-2D will be simulated applying both FOSM and Monte Carlo Simulations for uncertainty analysis.

II. UNCERTAINTY ANALYSIS

A. *First-Order Second-Moment (FOSM)*

- FOSM

The FOSM is given by the first order Taylor series expansion at the central values of the input variables, which is then truncated after the first-order term. Thus, if the variables are statistically independent the output variance is given by

$$\sigma_Z^2 = \sum_i \sigma_i^2 \left(\frac{\partial Z}{\partial p_i}\bigg|_{\mu_i} \right)^2 \quad (1)$$

where Z is the model output, p_i are the input parameters, μ_i are the mean values and σ_i^2 are the variances of the input parameters. All input parameters are considered here to be described by a Gaussian distribution, in which the variance represents the parameter uncertainty.

The partial derivatives of output Z with respect to parameter p_i in (1) has to be computed at the mean value μ_i of parameter p_i and can be calculated using Algorithmic Differentiation (AD)[14] up to machine accuracy (in contrast to numerical differentiation). The great advantage of using AD is that the derivatives of the model output with respect to an uncertain input parameter can be calculated by one single AD simulation. Several studies have been carried out with FOSM by means of AD ([4],[7],[10]), but there are still open questions regarding its applicability.

The drawback of the FOSM method lies on the linearity assumption. If deviations in the input parameters are not small enough, the output variance cannot be approximated well with the first-order terms in the series expansion. Since the partial derivative in (1) might change over the deviation interval considerably, both over– and underestimation of the true output deviation are possible.

- Compound FOSM (CFOSM)

Compound FOSM is an adaptation of the FOSM method for non-linear systems. Instead of considering a single value for the variance of each input parameter to represent its probability distribution, multiple values are taken into account. The Gaussian distribution of an input parameter with high variance is substituted by several Gaussian distributions with smaller variances. The weighted combination of the sub-distributions represents nearly the same distribution as the original one.

For a parameter p_i the mean value and variance of a compound distribution represented with j sub-distributions is given according to [11] by

$$\sigma_i^2 = \sum_j w_j (\mu_{ij}^2 + \sigma_{ij}^2) - \mu_i^2 \quad (2)$$

$$\mu_i = \sum_j w_j \mu_{ij} \quad (3)$$

where w_j are the weights of the sub-distributions, μ_{ij}, σ_{ij} are the moments of the sub-distributions for parameter p_i.

In CFOSM we define the variance of model output Z by combining (1) and (2):

$$\sigma_Z^2 = \sum_i \sum_j [w_j (\mu_{ij}^2 + \sigma_{ij}^2) - \mu_i^2] \left(\frac{\partial Z}{\partial p_i}\bigg|_{\mu_{ij}} \right)^2 \quad (4)$$

given i input parameters and j sub-distributions.

In CFOSM the uncertainty analysis has to be carried out for each member (sub-distribution) of the compound distribution (the partial derivatives have to be computed at the mean values μ_{ij} of the sub-distributions).

The number of sub-distributions (j), their mean values (μ_{ij}) and deviations (σ_{ij}) will affect CFOSM results. Therefore, the mean and the standard deviation of each sub-distribution should be chosen carefully, so that the original distribution is well represented.

In order to apply the CFOSM method, w_j, μ_{ij}, σ_{ij} must be defined. For given moments (μ_i, σ_i) of the original probability distribution (Fig. 1a), the number of sub-distributions (j) and their moments (μ_{ij}, σ_{ij}) must be defined

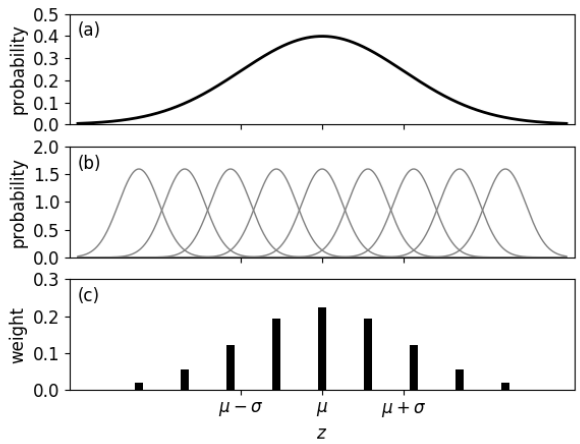


Figure 1*: Construction of a compound distribution.*

(Fig. 1b). After that, based on the cumulative density function of Fig. 1a, the partial areas relative to each sub-distribution (using the middle point between two successive μ_j) gives its corresponding weight (Fig. 1c). The final result for the compound distribution is then presented in Fig. 2.

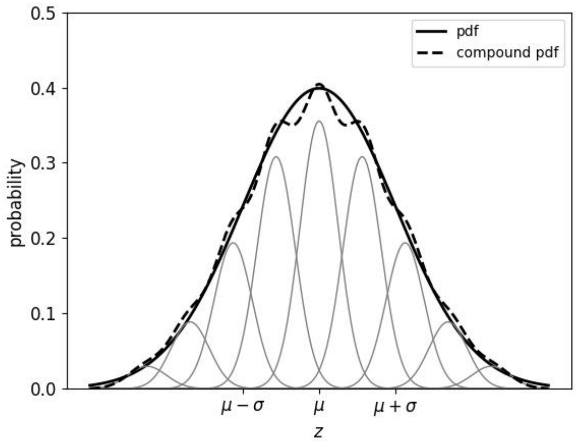


Figure 2: *Simple and compound probability distribution functions*.

B. *Monte Carlo Simulations (MCS)*

An alternative to the FOSM is to use the MCS approach for uncertainty analysis. A large number of model simulations (10^2-10^4) have to be carried out with different setups of uncertain parameters considered to be physically and statistically acceptable. Results will cover all possible outcomes if the statistical representation of input parameters is correct. However, this method requires much more computational effort and results might underestimate the true distribution of output values.

The confidence limits (CL) from the simulations can be derived from an empirical distribution function (EDF). From the cumulative EDF two points corresponding to the CL are chosen in order to get the function values. The absolute difference gives the CL.

The CL from the MCS method can be compared to FOSM and CFOSM results by calculating their corresponding CL as

$$CL_{FOSM} = 2 \cdot n \cdot \sigma_Z \quad (5)$$

where *n* is a factor corresponding to the level of confidence (e.g. *n*=3 means a 99% CL).

III. APPLICATIONS

A. *Analytical example*

An analytical function will be used as test case, in which the derivative can be exactly determined. If we take the function

$$f(x) = c \cdot \arctan(b \cdot x - a) + d \quad (6)$$

with derivative

$$f'(x) = \frac{b \cdot c}{(b \cdot x - a)^2 + 1} \quad (7)$$

then the graphical representation of *f(x)* and *f'(x)* at $x = \mu$ is shown in Fig. 3.

The FOSM method applied to *f(x)* provides a confidence interval of the function, based on the derivative of the output at the mean value of the inputs. The confidence interval itself is represented by the projection of the tangent on the ordinate axis (light red) multiplied by a deviation related to the parameter uncertainty.

In Fig. 4 the same function is presented, but now evaluated with the CFOSM method. Instead of using just one point to calculate the derivative and estimate the confidence interval, several points are selected around the original one. A smaller value for the parameter deviation is now defined, and the confidence interval is now obtained by projecting all tangents on the ordinate axis. The total interval length depends on the underlying model. For the analytical example the constant *b* in (6) determines the reducing factor. The interval length in Fig. 4 is finally smaller than the one obtained in Fig. 3 (see Tab. 1).

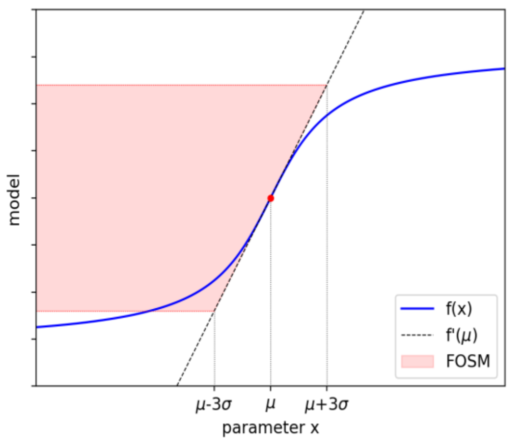


Figure 3: *FOSM concept applied to f(x).*

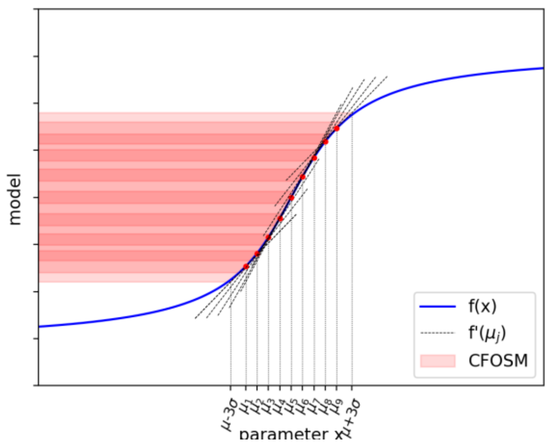


Figure 4: *CFOSM concept applied to f(x).*

TABLE 1: CONFIDENCE INTERVAL OF F(X).

x interval	f(x), b=1	FOSM	CFOSM
[μ-3σ , μ+3σ]	8.8	12.0	9.2

B. *The bump test case*

This test case also known as "bosse" is used as validation test case for SISYPHE, the sediment transport and bed evolution module from the Telemac-Mascaret Modelling System ([12],[13]). In the experiment a sinusoidal dune migrates during four hours due to a constant flow. The model topography is shown in Fig. 5.

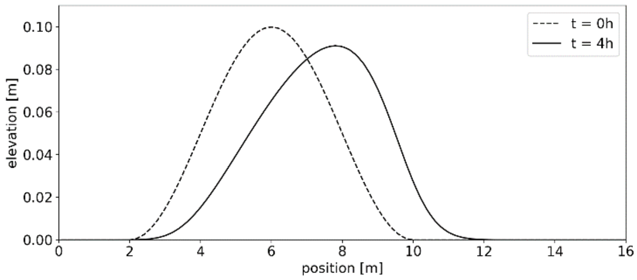


Figure 5: *Model topography.*

The parameters considered to contribute to the overall model uncertainty in this example are the bottom roughness, the slope effect and the median sediment grain size. The transport formula of Engelund-Hansen is applied. The bottom roughness is defined by the Strickler coefficient and the slope effect using the formula of Koch & Flokstra by the beta coefficient. The mean value μ and standard deviation σ for each parameter is presented in Tab. 2.

TABLE 2: STATISTICAL MOMENTS OF THE BUMP MODEL PARAMETERS.

	Median grain size (d_{50}) [m]	Roughness coefficient (k_s) [$m^{1/3}s^{-1}$]	Slope effect coefficient (β) [-]
μ	$3\cdot10^{-4}$	40	1.3
σ	$3\cdot10^{-6}$	0.5	0.3

The FOSM method is directly computed with AD in Telemac (Telemac-AD branch Foxface, based on Telemac-2D V7P2). Results from [9] already showed good agreement between the FOSM calculated and MCS methods. The new proposed method using j=9 and $\sigma_j = 0.25 * \sigma$ has been applied. Results from CFOSM also perform very similar to MCS with 1000 members, here presented for a 99% confidence interval (see Fig. 6).

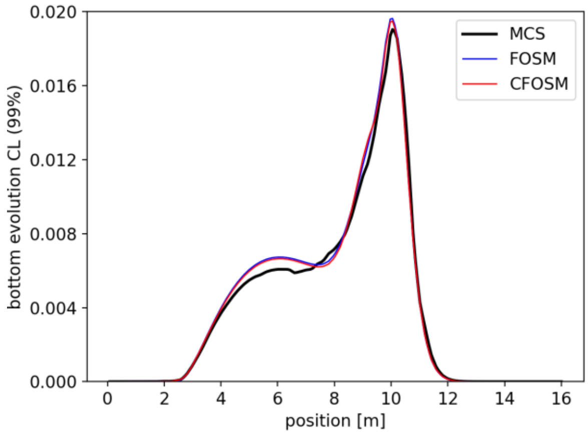


Figure 6: *Confidence limits of bottom evolution.*

Results presented so far do not add any improvement, as the linear approach already shows good agreement with the MCS method. With regard to computation times, FOSM (Telemac-AD) takes about 9 times longer than calculations with Telemac-2D for a single simulation. In total simulation time, FOSM took 2.7 min (1 distribution, 3 parameters), CFOSM 23.9 min (9 sub-distributions, 3 parameters) and MCS 100 min (1000 simulations).

However, a second test was carried out, in which a new set of parameters has been defined in order to consider more non-linearities (see Tab. 3).

TABLE 3: STATISTICAL MOMENTS OF THE BUMP MODEL PARAMETER SET 2.

	Median grain size (d_{50}) [m]	Roughness coefficient (k_s) [$m^{1/3}s^{-1}$]	Slope effect coefficient (β) [-]
μ	$3\cdot10^{-4}$	40	1.3
σ	$3\cdot10^{-5}$	4.0	0.3

In this second parameter set the median grain size and the roughness coefficient are considered to have a larger standard deviation, equals to 10% of the respective mean value. Results from the uncertainty analysis (see Fig. 7) differ among the three methods. Up to position 8 m the methods show a good agreement, but the peak around position 10 m happens before in FOSM and after in CFOSM. In general, assuming that the profile shape given by the MCS method is correct, the results of CFOSM approximate the true uncertainties better than FOSM. With respect to the number and deviation of the sub-distributions, a few tests showed that results differ very little for $j \geq 5$. However, the chosen standard deviation should be chosen accordingly. Therefore, further testing is still necessary on this topic.

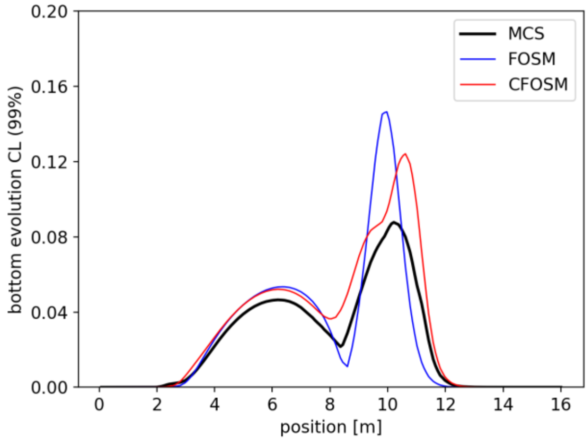


Figure 7: *Confidence limits of bottom evolution for parameter set 2.*

C. *The flume experiment test case*

In this example the new method can be tested in a less theoretical case. The numerical model is designed based on the experiment of [5], a 180° channel bend with a constant radius of curvature. The experiment is conducted during almost 6 hours with unsteady flow given by a hydrograph (see Fig. 8). The initial bottom is flat with a small slope downstream and it develops to a typical cross-section with sediment deposition near the inner side along the channel bend (Fig. 9). Also this example is used as validation test case for SISYPHE.

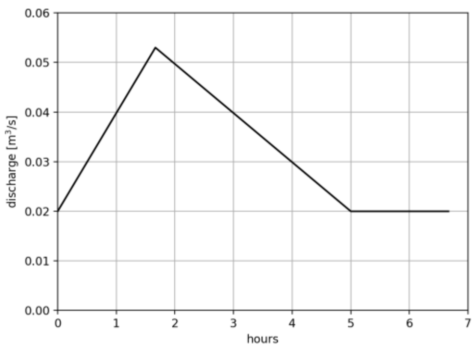


Figure 8: *Hydrograph used in the flume experiment.*

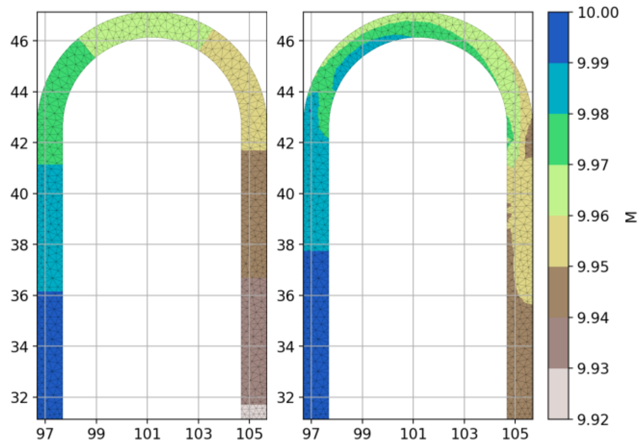


Figure 9: *Initial (left) and final (right) model topography.*

In this test case the same input parameters as in the bump test case have been considered, and additionally the α parameter related to secondary currents is taken into account. The transport formula of Meyer-Peter and Müller is applied and the roughness coefficient is defined after Nikuradse. In Tab. 4 the mean and standard deviation from each parameter are given.

TABLE 4: STATISTICAL MOMENTS OF THE FLUME MODEL PARAMETERS.

	Median grain size (d_{50}) **[m]**	**Roughness coefficient (k_s)** **[m]**	**Slope effect coefficient (β)** **[-]**	**Secondary currents coefficient (α)** **[-]**
μ	$1 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	1.3	1.0
σ	$1 \cdot 10^{-4}$	$3 \cdot 10^{-4}$	0.3	0.1

Similarly to the previous test case, the CFOSM method has been applied using j=9 and $\sigma_j = 0.25 * \sigma$. The results from the uncertainty analysis are shown in Fig. 10. The confidence limits from the MCS with 1000 members indicate higher uncertainty at the outer side and at the exit from the bend on the right side (in flow direction). At the center of the flume along the bend results present a smaller deviation.

In general, the FOSM confidence limits agree well with the MCS results. Along the outer side, however, FOSM clearly underestimates the uncertainty. FOSM results before and after the bend are very similar to MCS results. With regard to computation times, FOSM (Telemac-AD) takes about 10 times longer than calculations with Telemac-2D for a single simulation. In total simulation time, FOSM took 20.5 min (1 distribution, 4 parameters), CFOSM 184.2 min (9 sub-distributions, 4 parameters) and MCS 516.7 min (1000 simulations).

The CFOSM confidence limits also agree qualitatively well with MCS results. Along the outer side CFOSM performs better than FOSM, and it produces an overall larger uncertainty.

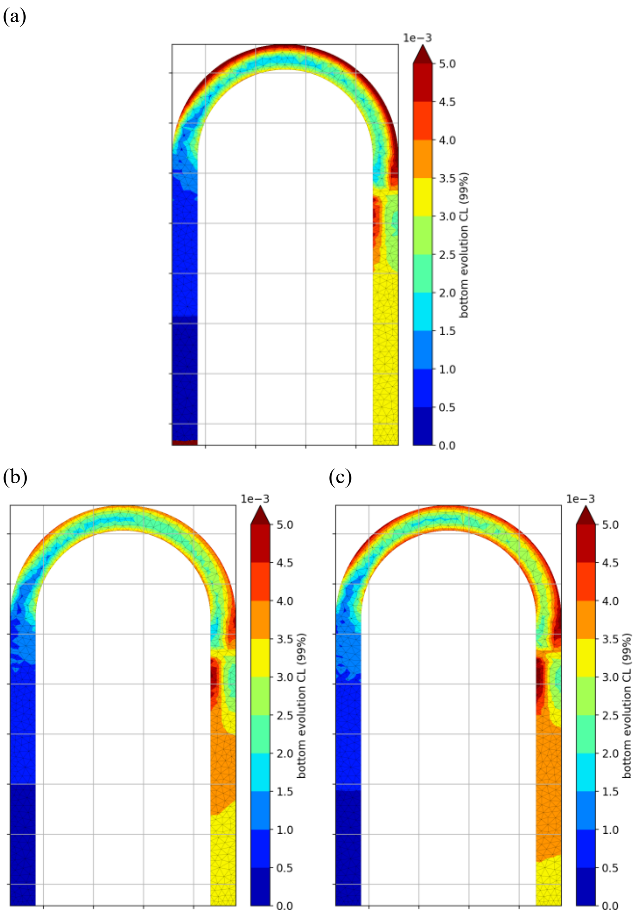
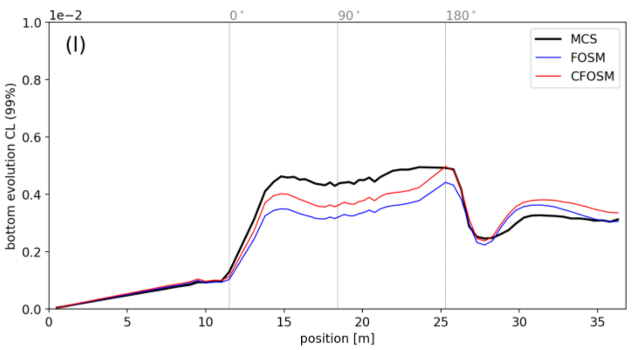


Figure 10: *Confidence limits (99%) of bottom evolution from the (a) MCS, (b) FOSM and (c) CFOSM methods.*

In order to have a clearer comparison among the three methods, a similar analysis to the bump test case has been carried out. For that, three profiles have been defined along the flume to evaluate the final bottom evolution (after 5.5 h): one at the center, one 40 cm to the left and one 40 cm to the right (Figure 11).



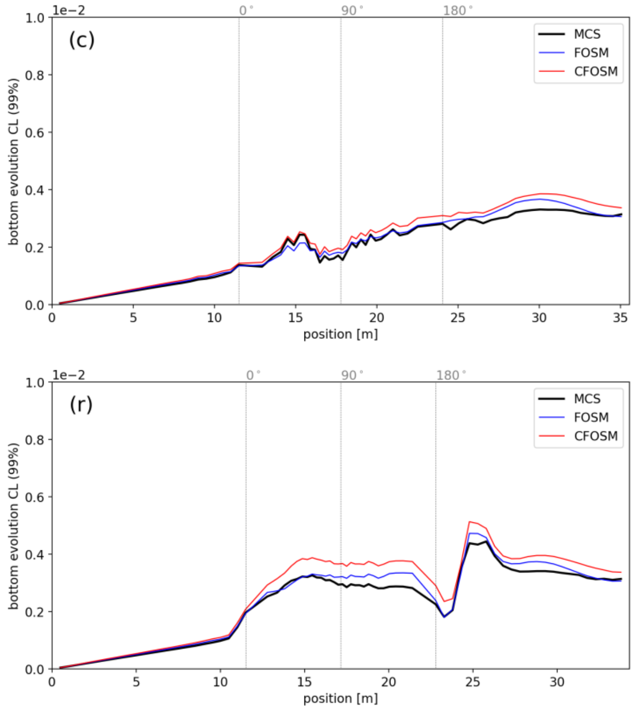


Figure 11: *Confidence limits of bottom evolution along the flume: (l) left, (c) center and (r) right profiles.*

Through this analysis it becomes clear that results are very similar before (0°) the bend among the three methods. Along the bend, FOSM agrees very well with MCS along the center and right profile, but shows a smaller uncertainty along the left profile (outer side). CFOSM reveals higher uncertainties at the center and right profiles, whereas at the left profile it gives a closer estimation to MCS along the bend.

IV. Discussion

In the analytical example (section III.A), the advantages of the CFOSM concept have been verified. The main idea is to improve the FOSM method and make it more robust for highly non-linear models and larger input variances.

In the bump test case (section III.B), results from the first simulation indicated that the proposed method does not improve the analysis of uncertainties. By considering larger deviations for the median grain size and bed roughness, however, new results showed a different situation. Because the first set of parameter deviations was relatively small, producing a quasi-linear variation in the bottom evolution, the use of the FOSM was good enough. In the second test, the larger deviations in the parameters led to a non-linear variation in the bottom evolution, which could not be fully determined by a single derivative. The CFOSM method indicated qualitatively better results taking the MCS method as reference, but with the benefit of computational costs 3 to 4 times lower.

Results from the flume experiment (section III.C), at first sight, indicated an overall increase in the confidence limits from the beginning until the end of the flume. This makes perfectly sense, as on a river usually downstream morphodynamic conditions depend on upstream conditions. Results before the bend given by the three methods agree very well, most probably due to linear and quasi-linear conditions found at those regions. Along the bend non-linear processes are probably dominant and should not be neglected.

V. Conclusion

A new uncertainty analysis method based on the first-order second-moment (FOSM) was proposed for non-linear processes. The compound FOSM (CFOSM) method was compared to FOSM and MCS methods.

The results from three test cases – an analytical, a bump and a flume bend – provided an insight on suitable conditions for using FOSM and CFOSM uncertainty analyses. According to those results, CFOSM showed its potential in the first two tests, but did not produce convincing better results in the 2D case. Although FOSM might work when dealing with small parameter deviations, it cannot approximate the true confidence interval of non-linear processes well.

Finally, there are still some open questions regarding the CFOSM method, such as the definition of the number of sub-distributions and their standard deviations, the performance of the method under more complex conditions, and covariance effects among parameters. Possible further development and tests still need to be discussed.

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