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***Abstract* — Using reliability analysis in morphodynamic simulation should be seen as a standard proceeding in project work. Due to deficient description of the physical processes, natural variability or imprecision of model parameters morphodynamic simulation becomes uncertain through highly sensitive model parameters. The sensitivity of these model parameters should be determined and their contributions to the variance of the model results should be quantified.**

Reliability analyses are compared by using three methods: a simple Scatter Analysis, a Monte Carlo method specialised to confidence limits and a first order method based on tangent-linear algorithmic differentiation (AD) of TELEMAC / SISYPHE. Showing the advantages of each method, different applications were used either from flume experiments or from project work. The influence of either wide spread or high sensitive input parameters could be estimated as well as areas of higher and lower uncertainty. Unfortunately all methods have relevant drawbacks applying in project work. Some new ideas are presented to overcome these limitations.

Moreover, a first example of automatic calibration of model parameters is shown. For that, an adjoint model of TELEMAC / SISYPHE was generated by the AD-enabled NAG Fortran compiler.

I. Introduction

In the last few years bed load management for the purpose of creating a dynamic bottom balance in federal waterways has increased significantly in importance. Numerical simulations of morphodynamic processes become an essential tool for bed load management. But these tools incorporate a lot of uncertainties due to unknown initial and boundary conditions, the natural variability or the imprecision of model parameters and the deficient description of the complex physical processes. Morphodynamic tasks are mostly connected to large scales and long term periods. Therefore the demand for calibration and validation increases as well as the uncertainty of model predictions. Evaluation and careful interpretation of numerical results are needed. Reliability analysis can be helpful with that, as it quantifies the uncertainties in time and space as well as according to its source.

Several sources determine the overall uncertainty of a numerical model. Most of them cannot be influenced by the user of a numerical program, except for the input parameters. It is well known that the range of model parameters accepted in literature can be quite huge. Therefore the influence of uncertain input parameters to morphodynamic model results is considered in this article. The advantage of using even a quite simple reliability method shall be shown. The effect of uncertain input parameters to the bottom evolution as the main result of the morphodynamic simulation is investigated. Instead of just one value for the bottom evolution in space and time a most probable value and a certain range, equivalent to the confidence interval can be given.

Many parameters of simulations processes must be estimated in advance. Calibrating the model parameters based on observations taken from measurements can be done by solving a least squares problem, where the sum of squared errors between observations and simulated values is minimised. Gradient based methods might be used to solve these problems, if gradients of the residual with respect to the parameters can be computed efficiently. Reverse mode AD can be used to create an adjoint model of the simulation, which can compute a gradient by just one adjoint model evaluation independent of the number of parameters to calibrate. A first adjoint model of TELEMAC / SISYPHE generated by the AD-enabled NAG Fortran compiler was used successfully to calibrate a set of parameters for a first example.

II. Reliability Methods

Three reliability methods and a method for automatic calibration based on algorithmic differentiation were applied for a project or two different flume experiments.

A. Scatter Analysis

The Scatter Analysis is a first order method. Therefore it is only adequate for linear or slightly non-linear problems. From the root mean square (RMS) the deviations are assumed. The RMS can be calculated from the first derivative multiplied by the standard deviation. When calculating the confidence limits only the first order terms are taken into account. The confidence interval of the evolution for a 68 % probability is two times the RMS and for a 95 % probability 4 times the RMS. For a detailed description please refer to [1].

The RMS of the state variable evolution E, which describes the bed level changes e.g. in a river, influenced by the friction coefficient ks with a Gaussian distribution, can be calculated as:

$$rms(E) = \frac{1}{2}\left[E(ks_0 + \sigma) - E(ks_0 - \sigma)\right] \quad (1)$$

$E(ks_0 +/- \sigma)$ are results from two simulation runs with $ks_0+\sigma$ and $ks_0-\sigma$, while σ is the standard deviation of ks and ks_0 the mean value. The calculations of the deviations or the confidence intervals of the bed level changes E for n uncertain parameters need only n*2 + 1 simulation runs [2].

Deciding whether a linear method is valid, the distortion for the evolution E can be used:

$$\delta E = \frac{1}{2} E''(ks_0)\sigma^2 << rms \quad (2)$$

The distortion can be calculated with the second derivative of E (E'') concerning an uncertain parameter (in this case ks) and the standard deviation of this parameter. In case of a linear function of E, the second derivative would be zero. The distortion can be used as an indicator for linearity. It should be much smaller than the RMS, otherwise the function is not slightly non-linear and the method is not adequate for this special problem. However, the distortion can only be used as an indicator for slight non-linearity in case of symmetric distributions.

B. Monte Carlo CL and Metamodel

The MC-CL method is a specialized Monte Carlo method which focuses on the confidence limits. It is not limited to linear problems and determines the confidence limits approximately while using as few as possible simulations. In case of strong non-linearities the confidence limits cannot be deduced from the root mean square (RMS) any more. Moreover it is not possible to calculate the RMS from the deviations. A connection between the confidence limits and the root mean square only exists in case of non-distorted Gaussian distribution as in linear functions. For strong non-linear functions the root mean square and the confidence limits are not equivalent, not proportional and furthermore there is no functional connection between them. A more detailed description of this method can be found in [1], [3].

All Monte Carlo methods require a large sample number for precise determination of the confidence limits and need even more samples for the probability density function. In order to reduce the number of required samples and / or increase the precision, a computationally efficient interpolation (metamodel) can be used. Such a model can be constructed using a moderate number of simulations. Afterwards a huge number of model results can be created by the metamodel. With these results the confidence limits and the probability density functions (PDF) can be found with a higher precision. The metamodel is using radial basis functions. For details refer to [4] and [5]. The used simulations for constructing the metamodel should be chosen in such a way, that the whole parameter space is covered as even as possible. As for the MC-CL method a generator is used to create the parameter set. In order to guarantee an optimal construction of the metamodel a uniform distribution of each parameter must be assumed.

C. First Order Reliability Method with Algorithmic differentiation

First-Order Reliability Method (FORM) is a linear method, successfully used in structure analysis (see for example [6] or [7]. As for the Scatter Analysis the wanted deviations of the results are calculated from the first derivative (more precisely these first order derivatives forms the so called Jacobian) multiplied by the vector of standard deviations of the uncertain parameters. These Jacobian – vector – products can be computed efficiently by a so called Tangent-Linear Model (TLM) of the original simulation. A TLM can be generated by Algorithmic Differentiation (AD) [8, 9]: AD tools transform the original simulation into a TLM by instrumenting the model with additional code, that allows to compute the desired Jacobian projection almost automatically.

For TELEMAC-2D and SISYPHE a TLM was created by the AD-enabled NAG Fortran compiler [10], a joint effort of the Software and Tools for Computational Engineering Institute (STCE), RWTH Aachen University, the University of Hertfordshire, and the Numerical Algorithm Group Ltd., Oxford, UK.

D. Automatic calibration based on Algorithmic Differentiation

Model calibration tries to improve the quality of the simulation by modifying parameters in such a way, that results known from experiments are reproduced by the simulation. These data, called “observation” or “truth”, can be generated by real world measurements, or by using results of other simulations, or even by the simulation system itself. Using the simulation itself can of course not verify that the simulation will match what happens in the real word. But it will give interesting insights in the behaviour of the simulation and can be used to test the chosen optimisation algorithm.

Starting from an initial set of parameter values (not necessarily valid), an optimisation problem can be formulated (twin experiment): Minimise the sum over the squares of all errors between the simulation results of the current parameter set and the observations plus an optional regularisation term (not required in our experiment). Note that there is no guarantee that the original parameter set can be found again: Other valid parameter sets can exist with results matching the observations closely. However the chosen optimisation method and the initial parameter set have strong influence on the result of the calibration.

With the adjoint model of TELEMAC / SISYPHE generated by the AD-enabled NAG Fortran compiler gradient based methods can be used to calibrate parameters of experiments. An adjoint model can compute a gradient of a scalar valued function (like the sum of error squares above) in one sweep at a fixed multiple of the runtime of the original problem (relative costs). The gradient is a vector whose elements are the sensitivities of the output value with respect to the individual input parameters. Increasing the number of parameters does not increase the relative costs required to get the gradient. In contrast, the computational effort of approximating the gradient with finite differences or computing the gradient with a tangent linear model depend directly on the number of parameters.

Note that the adjoint model is in development state, thus only small examples can be handled at the moment. Ongoing work on the adjoint model (checkpointing, parallelism, special handling of linear solvers etc.) will increase the possible problem size dramatically.

III. Applications

Since about 10 years BAW deals with reliability analysis for morphodynamic models mainly within a research and development project. In the following some applications are shown from flume experiments and from project work. The advantages of each method are presented as well as the drawbacks.

A. *Reliability analysis in project work – River Rhine model*

For a 60 km long stretch of river Rhine from Iffezheim to Speyer TELEMAC-2D coupled with the morphodynamic module SISYPHE and the dredging module DredgeSim was applied. A historical hydrograph of 10 years was simulated to calibrate the model including artificial bed load supply and dredging activities. Such long term simulations incorporate a large scope of natural and numerical uncertainties. From the experiences gained during the calibration 9 parameters were assumed to be uncertain: The active layer thickness, the pre-factor of the Meyer-Peter Mueller formula, the parameter of the slope effect of Koch & Flokstra, the parameter for the secondary current approach, the sieve line including the mean grain size of the transported material and of the artificial bed load supply and the Nikuradse roughness coefficient of three different zones (river channel, bank area, groynes). The corresponding formulas for all parameters can be found in [11]. The three most sensitive parameters are the active layer thickness, the friction coefficient of the river channel and the parameter for the slope effect. For the reliability analysis the Scatter Analysis, the MC-CL and the metamodelling (not presented here) were chosen. Unfortunately the FORM method with algorithmic differentiation could not be compared. The incorporated module DredgeSim is not in the AD version yet. A detailed description of this reliability analysis can be found in [12].

Fig. 1 shows the 68% deviation of the bottom evolution according to the river channel friction coefficient.

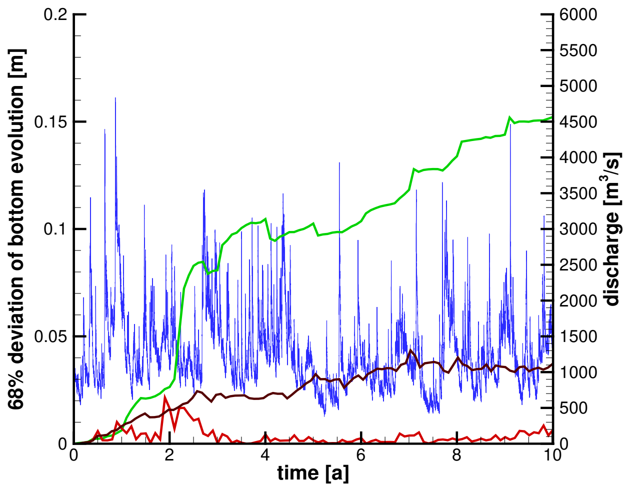

Figure 1. 68% deviation of the bottom evolution according to the river channel friction coefficient calculated with the Scatter Analysis for 10 years (green: mean value for the whole model area, red: representative point in the river channel, brown: averaged value for the fairway without disposal areas, blue: discharge).

A Gaussian distribution for this friction coefficient is assumed with a mean value of 2 cm and a standard deviation of 1.33 mm. With the Scatter Analysis a period of 10 years could be analysed. The green line represents the mean value for the whole model area. The red line is the product of just one node, a representative one, in the river channel. And the brown line contains an averaged value for the fairway excluding some disposal areas, which have enormous uncertainties. Generally the mean value for the whole model area increases over the time (Fig. 1 green line). Only in some rare occasions it decreases. The increase of uncertainty is higher during smaller discharges (e.g. low water conditions during the 3rd year). It seems that declines mostly occur during high water conditions. Contrarily to the assumption that the uncertainty is proportional to the amount of sediment transport (at least in this example), high water conditions lead to a state of the system which is more independent of the parameters. This has to be verified further. Unfortunately the averaged 68% deviation didn't reach a maximum level even over such a long period, but follows a trend. On the other hand the local deviation at some point in the river channel as well as the averaged value over the fairway excluding the disposal areas has indeed a maximum level and no trend. As expected, the overall uncertainty increases with time and long term simulation should be analysed very carefully. Nevertheless for some parts the local deviations reach a maximum and afterwards level around a mean value (e.g. in the river channel, Fig. 1 brown line). This means, that the presented model can be used for long term prediction without losing a certain confidence interval.

The assumption of linear system behaviour is probably not valid for such long time periods. So far all methods for non-linear system behaviour used at BAW are based on Monte Carlo simulations. All these methods need enormous amount of computing time. For this reason a comparison between the SA and the MC-CL is made for a shorter period. Fig. 2 shows the 95% deviation of the bottom evolution for the first 17 months. For the first 5 months both methods come to the same results. Afterwards only a qualitatively agreement exists. The SA overestimates the values clearly with increasing tendency. Nevertheless due to the qualitative compliance it can be assumed, that also with the MC-CL the deviations will not increase infinitely but reach a certain level.

For the project both methods are not completely satisfying. The Scatter Analysis loses comparably fast the validity due to strong non-linear system behaviour. For a Monte Carlo CL method at least 150 simulation runs were needed (better twice as much or more, see section B). For that 64 cores for approx. 130 days on a parallel compute server at BAW were used to simulate only 17 months. But for morphodynamic tasks simulations for much longer time periods like decades are of interest. The needed computing time is still not available for project work.

B. Comparison MC-CL and FORM with AD – Sisyphe validation test case "BOSSE"

The validation test case of SISYPHE called "BOSSE" is used to show the differences between FORM with AD and MC-CL. In this experiment a sinusoidal dune is moved 4 hours due to a constant flow. The simulation is done with SISYPHE stand-alone. Further details can be found in the SISYPHE validation document [13]. The influence of the

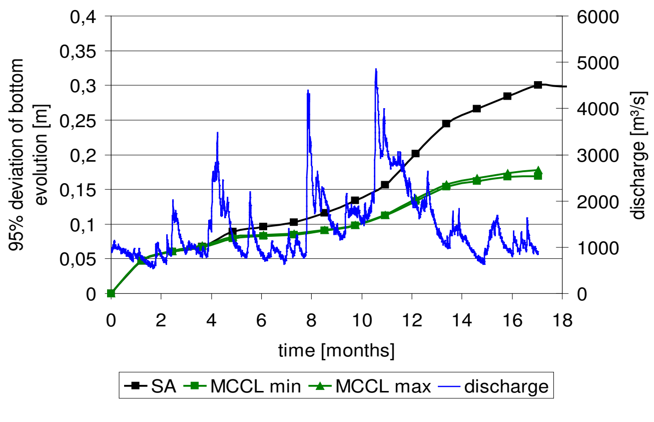

Figure 2. Comparison of the 95 % deviation of bottom evolution calculated with the Scatter Analysis and MC-CL.

roughness coefficient (Strickler) and the slope effect (parameter beta in Koch & Flokstra formulation) is investigated. A Gaussian distribution is assumed for both input parameters.

The Strickler value had a mean value of 40 $m^{1/3}/s$ with a standard deviation of 0.5 $m^{1/3}/s$, the dimensionless parameter beta had a mean value of 1.3 with a standard deviation of 0.3. With these distributions the effect to the bottom evolution is about the same for both parameters. The standard deviations were set to small values in order to stay into a range with slightly linear system behaviour.

Fig. 3 shows the 95 % deviation of bottom evolution in respect to the Strickler and the slope effect parameter calculated with FORM and MC-CL with 100 and 1000 simulation runs. Assuming, that the MC-CL with 1000 simulation calculates the best results, the linear method matches the results quite well. Interestingly the FORM results match even better than the MC-CL with only 100 simulation runs. The differences are strongest at the stoss-side of the dune, where the maximum slope is located.

For the MC-CL the CDF (cumulative distribution function) is approximated with an EDF (Empirical Distribution Function). The corresponding error err_{CDF} is dependent on the number of experiments N_{exp} and the confidence level α. It can be calculated with

$$err_{CDF} = \sqrt{\frac{(1-\alpha^2)}{4N_{exp}}} \tag{3}$$

if the number of experiments is much higher than $2/(1-\alpha)$.

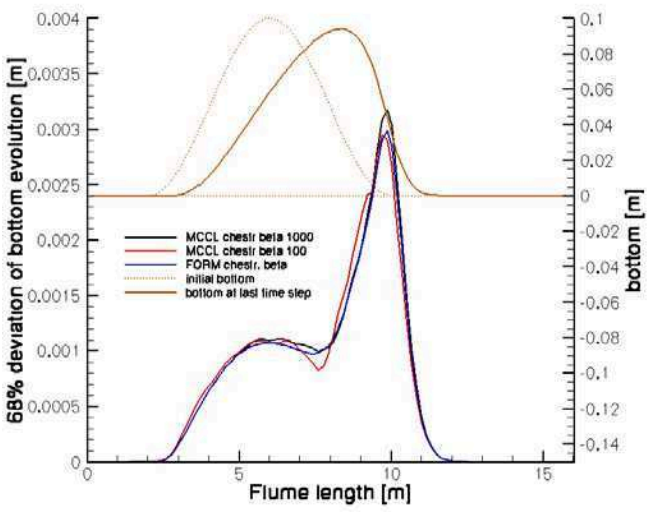

Figure 3. Comparison of the 68 % deviation of bottom evolution calculated with MC-CL using 100 (red line) and 1000 (black line) simulation runs and with FORM (blue line).

A confidence level of 68 % needs much more simulation runs than 40. For the shown 68% deviation and 100 experiments an error of 0.037 is gained. With 1000 simulations the error reduces to 0.012. From this example it must be derived that either the number of 100 simulation runs is not sufficiently higher than 40, or that an error of approx. 4 % is not satisfying. This leads to even higher numbers for the MC-CL method, which is often not possible for project work.

C. Comparison MC-CL and FORM with AD - Laboratory experiment with 180° bend

Another validation case which tests the effect of secondary currents is the experiment of Yen and Lee [14] in a flume with a 180° bend. In this experiment an unsteady flow discharge modifies the initial flat bottom to a typically cross section with an outer and inner bank. Starting from an initial flow rate of 0.02 m^3/s (corresponding to incipient motion), the flow discharge is linearly increased during 5 h up to 0.053 m^3/s and then progressively decreased back to its initial value. The results of the coupled hydrodynamic / morphodynamic model are reasonably satisfying for a depth averaged model (see [15]). For a further calibration the sensitivities of the bed level changes concerning the input parameters were conducted. Exemplarily the effect of a Gaussian distributed roughness coefficient to the bed evolution is chosen. The mean value of the roughness coefficient of Nikuradse was set to 3 mm with a standard deviation of 0.1 mm. The sensitivities were calculated with the AD version of SISYPHE and TELEMAC-2D v6p0 and the MC-CL method with 1000 simulation runs. The AD-model needed approx. only 0.7 % of the computing time of 1000 MC-CL simulation runs. This illustrates very clearly the big advantage of the AD based FORM method. Fig. 4 shows the comparison of the 68% deviation of bottom evolution according to the roughness coefficient for both methods after 5 hours.

The results of both methods match qualitatively and quantitatively well. Nevertheless there are some higher local differences at the side walls (see Fig. 5). These originate from locally high deviations that were calculated with both methods, but not exactly at the same position. The assumed variation of the roughness coefficient from 2.7 to 3.3 mm is comparably small. As expected the resulting deviations after 5 hours simulation are small too. For most points the 68% deviation is less than 1/100 of the maximum bottom evolution. The locally high deviations suggest some strong non-linear system behaviour or some simulation instability, which intensify for the deviations. Both methods predict them at slightly different places and they occur immediately and not after some time. Again it seems that both methods are not optimal to give reliable values for the deviations respectively the confidence intervals.

Nevertheless some important assumptions can be drawn from the calculated deviations: The influence due to such a small roughness change is small compared to the bed level

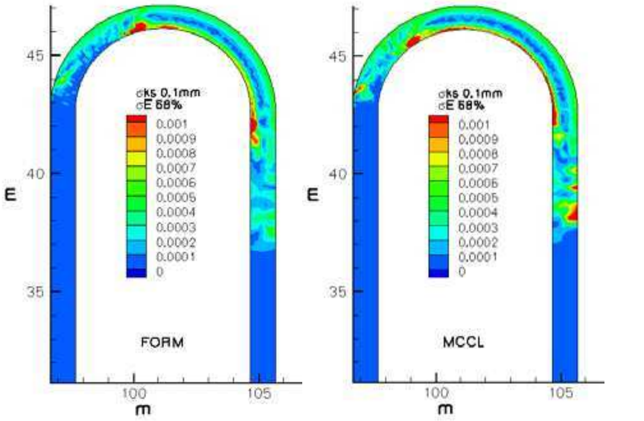

Figure 4. Comparison of the 68 % deviation of bottom evolution according to the friction coefficient calculated with FORM and AD (left) and MCCL (right).

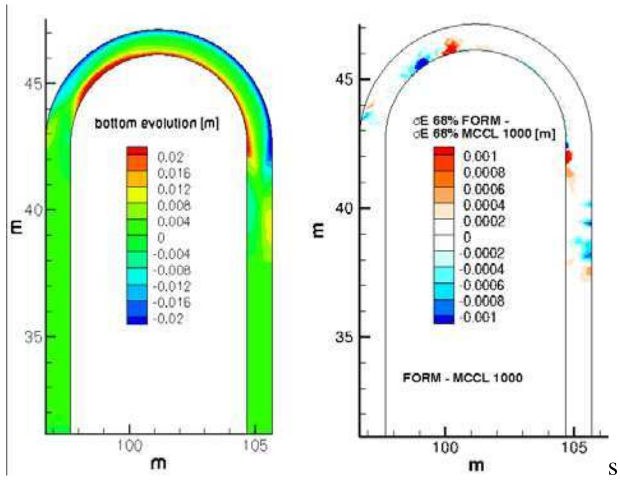

Figure 5. Bottom evolution calculated with the mean value of the roughness coefficient (left) and differences of the 68 % deviation of bottom evolution according to the friction coefficient between the MCCL and FORM based on AD (right).

changes. At the inner part of the channel the simulation is far less uncertain than at the boundaries. This means that the mean bed level change can be predicted much better, than the cross slope.

D. Automatic calibration based on AD – Sisyphe validation test case "BOSSE"

For a first calibration test at STCE the SISYPHE validation test case "BOSSE" was modified to support a zonal model for the Strickler roughness coefficient *kst*. Instead of one scalar value for all grid nodes, the roughness coefficient was set for all grid nodes by a special designed function *kst(p)* taking an input vector $p \in R^{92}$ of 92 input parameters.

Looking at SISYPHE as a function $E_{kst}(p)$: $R^{92} \rightarrow R^{891}$ that maps first an input vector p according to $kst(p)$ into roughness coefficients of all grid points, and then computes the bottom evolution $E_{kst}(p) \in R^{891}$, SISYPHE was used to compute the observations $E^{obs} = E_{kst}(p^{obs})$. The parameters p^{obs} were chosen in such a way, that 48 roughness zones were created by $kst(p^{obs})$ as shown in Fig. 6.

A least squares residual functional was defined for arbitrary input vectors $p \in R^{92}$ as

$$g(p) = \sum_{i=1}^{891} \left(E_{kst,i}(p) - E_i^{obs} \right)^2 \cdot w_i \tag{4}$$

with weights $w_i = 10^5$, that measures the error in the bottom evolution for an input vector p. The optimisation method BFGS (Broyden-Fletcher-Goldfarb-Shanno) from the Python - package SciPy (www.scipy.org) was used to solve the minimisation problem

$$\min_{p \in R^{92}} g(p) \tag{5}$$

The algorithm requires two functions: One to evaluate the value of $E_{kst}(p)$, and another to compute the gradient of $E_{kst}(p)$ with respect to the input parameter p. The gradient is used to determine a search direction; the evaluation of E_{kst} is used to decide on the step length along the direction given by the gradient. The evaluation of E_{kst} is done by just calling SISYPHE, whereas the gradient is computed via the adjoint model of SISYPHE generated by the AD- enabled NAG Fortran compiler.

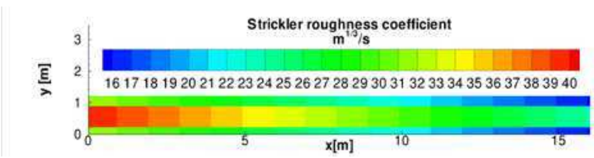

Figure 6. 48 roughness coefficient zones for optimisation problem.

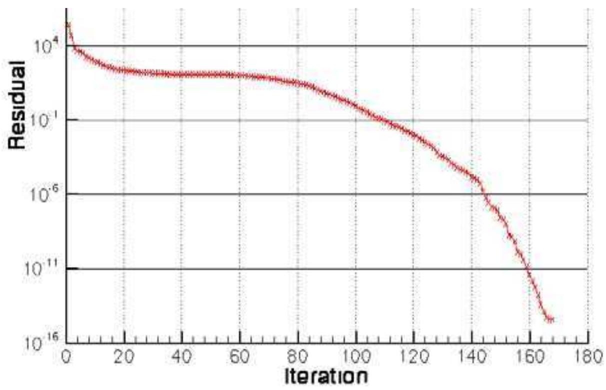

Figure 7. Development of the residual.

Fig. 7 shows (in log scale) the development of the residual $g(p)$ starting from an initial guess p^0 for the parameter vector p such that $kst(p^0)$ gave a value of 80 for the roughness of all grid points. Thus the initial residual $g(p^0)$ was around 260,000. After 131 Iterations the norm of the gradient was reduced from roughly 2,300 to less than 0.1 (residual around 0.002), after 167 iterations the algorithm terminates with gradient norm below10^{-7}. The minimiser found matched the true parameter vector p^{obs} up to at least 8 decimal digits, the residual value was within the numerical noise (less than 10^{-14}). For a first try on automatic calibration these results are very promising.

To investigate more realistic calibration problems the adjoint model needs to (and will) be improved (checkpointing, parallelism, special handling of linear solvers etc.). Moreover problem specific optimisation routines need to be selected, implemented or even created. (For instance, the optimisation given above should not be unconstrained, since a Strickler roughness coefficient below zero or above 100 does not make sense).

IV. DISCUSSION OF APPLIED RELIABILITY METHODS

The applied reliability methods are not satisfying, while they have all relevant drawbacks if it comes to project work. The possibility to get reliable quantitative statements from linear approaches like FORM or Scatter Analysis decreases very fast with simulation time.

On the other hand all applied non-linear methods are based on Monte Carlo simulations. The big disadvantage is the needed huge number of simulation runs. The required computing time is simply not available. Model extents as well as simulated time periods are usually too high in project work. With new and faster computers model dimensions and time periods always increased in the past. For that reason it cannot be hoped to overcome this limitation of the Monte Carlo method only by increasing computer power. Hence non-linear methods based on algorithmic differentiation seem the more promising way. Some ideas are already scheduled for testing. AD can also provide second derivatives. This gives the possibility to apply a second order reliability method (SORM). Furthermore in AD a vector mode exists. With that multiple Jacobian projections can be calculated simultaneously. Furthermore with a newly implemented very precise restart option derivates can be calculated faster for different parameter sets. Each derivative would be still linear, but the analysis space can be enhanced.

V. CONCLUSIONS AND OUTLOOK

In this paper three reliability methods have been applied to flume experiments and project work. Two linear methods, the Scatter Analysis and the first order reliability method (FORM) using algorithmic differentiation (AD) were compared to a specialised Monte Carlo method (MC-CL). For linear or slightly non-linear model behaviour the linear methods are very useful. However, most morphodynamic tasks are of long term and large scale. Both imply an increasing non-linear behaviour. With that model class only qualitative statements can be made. On the other hand Monte Carlo methods require such amount of computing time that it is simply not possible to conduct in project work. Further investigations for non-linear methods based on algorithmic differentiation seem most promising.

First results of automatic calibration using an optimisation due to algorithmic differentiation in adjoint mode have been shown. The quality of the calibrated parameter set was determined within the optimisation algorithm. This increases the prediction ability of the model respectively the model reliability.

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