**This highlight refers to the PhD Thesis by Yous van Halder (2022)**

# An adaptive minimum spanning tree multi-element method for uncertainty quantification of smooth and discontinuous responses

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## Background

Uncertainty Quantification (UQ) has become increasingly important for complex engineering applications. Determining and quantifying the influence of parametric and model-form uncertainties is essential for a wide range of applications, among which fluid dynamics.

A well-known sampling method for propagating uncertainties through a model is the Monte Carlo method. Despite its easy implementation and wide applicability, the Monte Carlo method suffers from slow convergence with increasing number of model evaluations when approximating the quantity of interest (QoI); it requires many samples for obtaining high-quality stochastic solutions. As an alternative to Monte Carlo methods, stochastic collocation (SC) methods were introduced, replacing the slow convergence of Monte Carlo methods by an exponential convergence rate. For a smooth QoI as a function of the uncertainties, fast convergence is achieved indeed with SC. However, if the QoI is highly non-linear or even discontinuous, Gibbs phenomena may occur, which deteriorate the accuracy globally. To avoid the occurrence of Gibbs phenomena, several alternatives to the SC methods were introduced, but they focus solely on discontinuous QoIs, leading to a significant increase in the number of samples needed for approximating smooth QoIs. As a remedy against this, the multi-element stochastic collocation (ME-SC) method was introduced. The idea of ME-SC is to decompose the domain, spanned by the uncertainties, into smaller non-overlapping sub-domains (called elements), in each of which the QoI is amenable for using an SC method. Gibbs phenomena still appear in the elements where there is a discontinuity in the QoI, but they are confined to these specific elements. Improving the multi-element approach is an active field of research and focuses on more efficient and robust domain decomposition. It is often unknown in advance if a QoI is smooth or non-smooth. Hence, choosing a method which is suited for either smooth or discontinuous responses is often not recommended.

## Method

We created a surrogate model, which works for both smooth and discontinuous QoIs and which requires no a-priori knowledge about the QoI. For this purpose, we proposed a novel domain decomposition method in combination with adaptive sampling for constructing the surrogate. The adaptive sampling procedure in our method is based on minimum spanning trees (MST), which add new sample points at places which are associated with a high probability density and/or where the QoI changes rapidly. The adaptively placed samples are classified and a support vector machine (SVM) is used to obtain a classification boundary, which serves as an approximation for the discontinuity location. This decomposition of the random space leads to elements on which each local QoI is amenable for interpolation without Gibbs phenomena. For constructing a surrogate model in each element a least orthogonal interpolant is employed, which is suited for interpolation on the scattered data points that we obtain with our adaptive sampling. Our method is abbreviated as MST-ME (minimum spanning tree multi-element) method. When assuming uniformly distributed probability density functions for the input parameters, the MST-ME method is also well suited to obtain a parametric solution of the partial differential equation (PDE) under consideration.

**Results**

We study the performance of the MST-ME method applied to a system of 1D conservation laws. This system consists of the 1D shallow water equations (SWEs), which describe the inviscid flow of a layer of fluid with free surface, under the action of gravity, with the thickness of the fluid layer small compared to the other length scales.

The initial condition for the system of PDEs is shown in the left graph of Figure 1. The solution of this Riemann problem can be computed exactly when working on an infinite spatial domain. The solution consists of two waves, a smooth one and a discontinuous one, travelling through the spatial domain, see right graph in Figure 1.

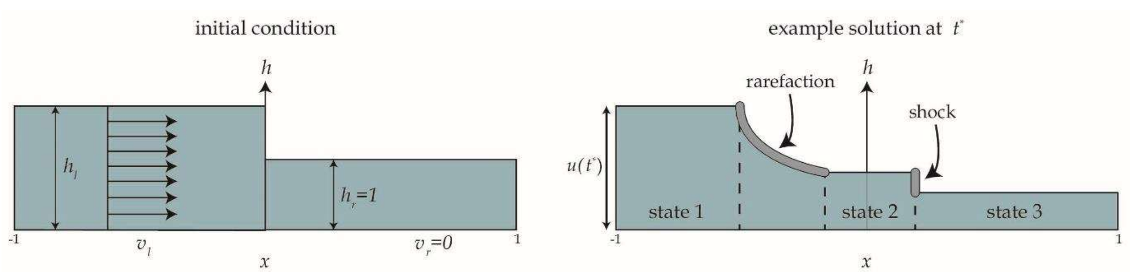


*Figure 1: Shallow-water test case.*

Solid-wall boundary conditions are imposed at $x = \pm 1$, and we employ a finite-volume method with an exact Riemann solver to compute the cell-face fluxes, and solve the SWEs using 256 finite volumes. An appropriate numerical method is used to integrate the SWEs in time and a ghost-cell method with respective properties is used for the boundaries. The initial left state ($h_l$,$v_l$) (Figure 1) is assumed to be uncertain and uniformly distributed. The uncertainty in the initial conditions is large to ensure that we get different characteristic behaviours of the QoI, which is defined as the fluid height at $x = -1$ at a certain time $t^*$.

Notice that the characteristics of this QoI will change significantly as time progresses. Either a transition between a shock and rarefaction wave, or a difference in wave speeds can result in a discontinuity in the QoI. This allows us to study the robustness of the MST-ME method, as this test case comprises both smooth and discontinuous QoI responses. We emphasize that the constructed surrogate for the QoI at time $t^*$ cannot be reused for other time instances, because the MST-ME method uses the QoI at the current time $t^*$ as a measure to place new samples.

The MST-ME method is used for the QoI at three different times, corresponding with a mildly non-linear (rather smooth), highly non-linear (rather non-smooth) and close to discontinuous QoI, respectively. The surrogate model and sample grids after 10 iterations are shown in Figure 2. The discontinuity in the QoI in the close to discontinuous case is caused by a shock wave (water jump), which hits the left boundary for certain values in the random space, but does not yet hit the left boundary for other values in the random space.

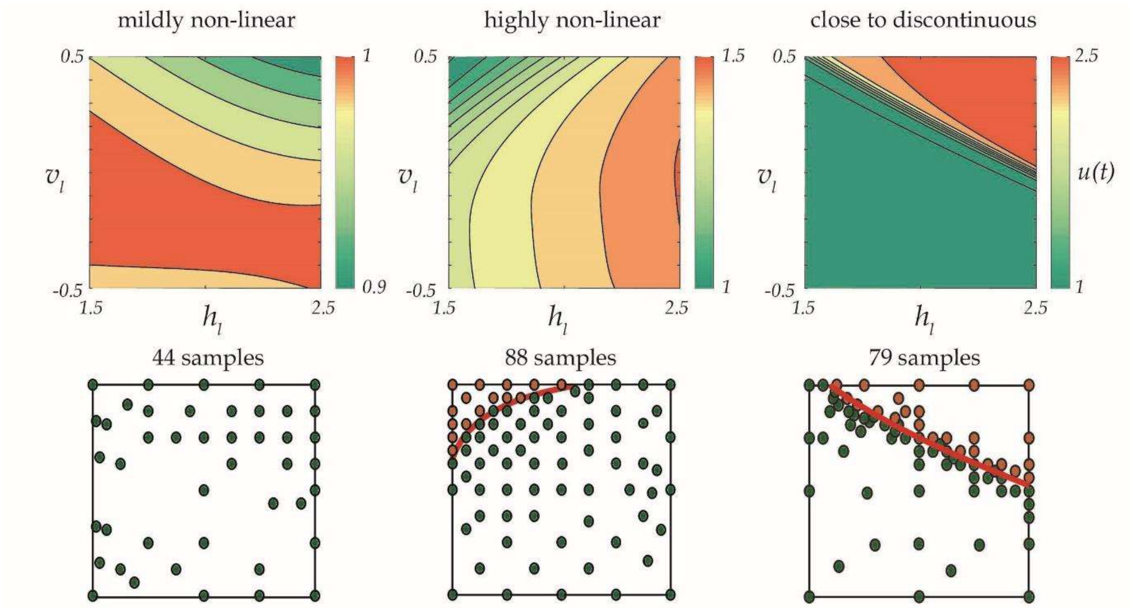


*Figure 2: The three QoI surrogate models and corresponding sample grids after 10 iterations.*

To investigate the accuracy of the MST-ME method, we determine the convergence. The error is based on $10^6$ Monte Carlo samples. The convergence of the $L_{2,\rho}$ error (see Van Halder et al., 2019) is shown in Figure 3. The results show that the error as a function of the samples decays fast for the mildly and highly non-linear case, as expected. The highly non-linear case shows a sudden drop in the error, which is caused by transition in the domain decomposition. First, the classification procedure detects a large enough jump in the sampled QoI to conclude that there is a discontinuity present in the QoI. As the MST-ME progresses, samples are added in the area of the possible discontinuity, until the jumps in the QoI values become small enough to classify the samples properly. This transition to a correct classification explains the sudden drop in the error for the highly non-linear case. MST-ME automatically detects the smoothness of the QoI, as the number of samples increases.

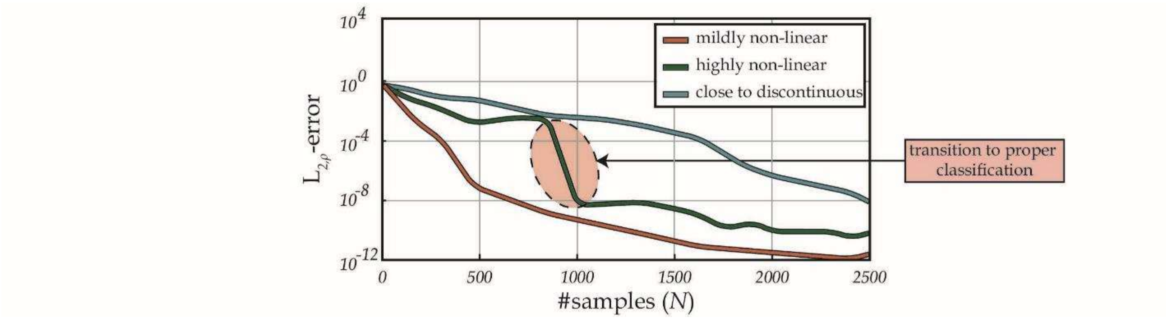


*Figure 3: Convergence of the MST-ME solution in the $L_{2,\rho}$-error.*


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**References**


Van Halder, Yous 2022. Efficient sampling and solver enhancement for uncertainty quantification, PhD Thesis, Eindhoven University of Technology.

Van Halder, Y., Sanderse, B., Koren, B. An adaptive minimum spanning tree multielement method for uncertainty quantification of smooth and discontinuous responses, SIAM Journal on Scientific Computing 41, A3624-A3648, 2019.