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Exploring complex models with metamodels: a way through the tangle?

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Research in the geosciences often necessitates application of simulation models to demonstrate the behaviour of complex systems, and there is now great variety in the types of model used across different disciplines. Despite this variety, however, such models typically employ many parameters of uncertain value, and the modelled system may itself be subject to many variable factors e.g. those controlling boundary and driving conditions. This creates a large, multi-dimensional factor space, which needs exploration if the full range of possible model outcomes is to be made evident. Also, although there have been great advances in computing power and model functionality over the last 25 years, each simulation may take hours or days to complete. Additionally, standard Monte Carlo or GLUE type simulation methodologies still require very large simulation run sizes to explore the factor space fully. Thus, potential computational burdens are very high, and a thorough factor space exploration usually becomes quite infeasible. Here we present a potentially highly efficient approach, based on statistically derived mediating functions called “metamodels”. These have been used extensively in engineering and operations research, and more complex “emulators” are gaining in importance as tools in some geoscientific disciplines (e.g. in climate research), but the metamodelling approach is generally not known or attempted in many studies. Using examples from geomorphology, hydrology and other subject areas, we show how a combination of "design of experiment" and regression analysis affords the possibility to derive metamodels for selected model output measures and output

times. Each metamodel comprises an equation formed of mathematical functions of the model input variables, and is thence used as a substitute for full model simulations. This permits rapid solution across the factor space, for any point and as many points of interest, with the inclusion as appropriate of associated error band estimates. The metamodels are also potentially shareable amongst researchers, yet retain the influence of the source model's complexity. In addition to covering matters related to experiment design, it is also hoped to show how the method can lead to interesting discoveries about modelled system behaviour.