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8 What has Global Sensitivity Analysis ever done for us? A systematic 9 review to support scientific advancement and to inform policy-making in 10 earth system modelling

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16 Abstract

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18 Computer models are essential tools in the earth system sciences. They underpin our search for understanding of earth system functioning and support 19 20 decision- and policy-making across spatial and temporal scales. To understand the implications of uncertainty and environmental variability on the identification 21 22 of such earth system models and their predictions, we can rely on increasingly 23 powerful Global Sensitivity Analysis (GSA) methods. Previous reviews have 24 characterised the variability of GSA methods available and their usability for 25 different tasks. In our paper we rather focus on reviewing what has been learned so far by applying GSA to models across the earth system sciences, 26 27 independently of the specific algorithm that was applied. We identify and 28 discuss 10 key findings with general applicability and relevance for the earth 29 sciences. We further provide an A-B-C-D of best practise in applying GSA 30 methods, which we have derived from analysing why some GSA applications 31 provided more insight than others.

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33 1. Introduction34

35 Computer models are essential tools in the earth system sciences. They 36 underpin our search for understanding of earth system functioning and 37 influence decision- and policy-making at various spatial and temporal scales. 38 For example, computer models of the atmospheric system are used to produce 39 short-term weather forecasts, which inform operational decisions at regional or 40 local scale, or to make long-term projections of the global climate, which forms 41 the basis of the international debate around climate change. Global hydrologic 42 models can now provide a coherent picture of hydrological dynamics across 43 our planet under past, current and potential future conditions (Schewe et al., 44 2014); while integrated assessment models integrate our climate system with 45 the socio-economic behaviour of society to assess the consequences of future policy scenarios (Stanton et al., 2009). Many other examples of the value of 46 47 computer models can be made for a variety of earth science areas, from 48 atmospheric circulation (Cotton et al., 1995) to biogeochemical processes in

49 the sea (Soetaert et al., 2000), from mantle dynamics (Yoshida and Santosh, 50 2011) to tsunamis impacts (Gelfenbaum et al., 2011).

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52 A key issue in the development of computer models is that they can guickly exhibit complicated behaviours because of the potentially high level of 53 54 interactions between their variables, and subsequently their parameters, even 55 when they only represent a relatively low number of physical processes. The 56 amount of internal interactions is destined to grow as we build models that are 57 increasingly more detailed and applied to larger domains. Two key factors are 58 boosting this process: the increasing availability of computing resources, 59 which enables the execution of models at unprecedented temporal and spatial 60 resolutions (Wood et al., 2011; Washington et al., 2012), and the increasing 61 availability of earth observations that can be used to force computer models 62 and evaluate their predictions (O'Neill and Steenman-Clark, 2002; Ramamurthy, 2006; Nativi et al., 2015). For example, Figure 1 shows the 63 increase in resolution and components of climate system models that was 64 65 made possible by the growth of computing power over the last decades. 66 67 Increasingly detailed computer models working at ever larger scales and finer 68 resolutions are expected to play a key role in advancing the earth system 69 sciences (Rauser et al., 2016; Wood et al., 2011; Bierkens et al., 2015), but this 70 growth in model complexity also comes at a price. As the level of interactions 71 between model components increases, modellers quickly lose the ability to 72 anticipate and interpret model behaviour and hence the ability to evaluate that 73 a model achieves the right response for the right reason (Beven and Cloke,

74 2012), i.e. that the model is consistent with the underlying 'perceptual model' of 75 system functioning (e.g. Klemes, 1986; Grayson et al., 1992; Wagener and 76 Gupta, 2005; Kirchner, 2006; Beven, 2007; Gupta et al., 2012; Hrachowitz et al., 2014). This issue is particularly problematic in earth system modelling 77 78 where incomplete knowledge of the system makes it impossible to validate 79 models simply based on fitting model predictions to observations. Oreskes et 80 al. (1994) therefore suggest that models should rather be evaluated in relative 81 terms, and model validation should consist in identifying the models that are 82 free from detectable flaws and that are internally consistent. Therefore, in the 83 remainder of this paper, we will rather use the term model 'evaluation' to refer 84 to any kind of model assessment or validation.

85

86 Another difficulty in the application and evaluation of earth system computer 87 models is that, even if internally consistent, their predictions may still be 88 erroneous as models are often forced by input variables that are only known 89 with a significant degree of uncertainty (McMillan et al., 2012). The difficulty is even greater for models with a large number of initial and boundary conditions, 90 91 for which measurements may be erroneous or simply unavailable. The problem 92 is sometimes seemingly mitigated by the growth in data products made 93 available by recent advances in earth monitoring (Butler, 2007) and 94 environmental sensing (Hart and Martinez, 2006). However, the translation of 95 raw measurements into data products usable for the modelling purpose (for 96 example, from a satellite measurement of soil microwave radiation to an

97 estimate of the soil water content) requires a set of pre-processing calculations
98 that constitute a modelling activity per se. As a consequence, distinguishing
99 between possible errors in the "main" hypothesis (the earth system computer
100 model) and other "auxiliary" hypotheses, such as the pre-processing of input
101 data used to force the model, can be difficult (Oreskes et al. 1994).

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103 Uncertainty about the forcing inputs of earth system models, and consequently 104 about their predictions, may have at least two other origins besides 105 measurement and pre-processing errors. One is the scarcity of observations 106 that still affects many areas of the world, either because regions are too remote 107 or because it is impossible to establish and maintain a reliable monitoring 108 network (Blöschl et al., 2013; Hrachowitz et al., 2013). The other is the shrinking 109 value of historical observations in a quickly-changing world (e.g. Jain and Lall, 110 2001). Traditionally many modelling studies have relied on the so called 111 'stationarity' assumption, i.e. the assumption that "natural systems fluctuate 112 within an unchanged envelope of variability" (Milly et al., 2008), when time 113 periods studied were not longer than maybe a few decades. This assumption 114 implies that observations collected in the past can inform the construction of 115 computer models that are intended to predict future conditions. The assumption 116 is hardly acceptable in a world where human activities are exerting an 117 unprecedented influence on natural systems leading to unprecedented rates of 118 environmental change (Crutzen and Stoermer, 2000). As socio-economic and 119 technological changes are largely unpredictable, they introduce significant uncertainty about future properties of the earth system and dramatically limit 120 121 our ability to make quantitative predictions about its evolution (Wagener et al., 122 2010)

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124 Lack of transparency about the scope of validity, the limitations and the 125 predictive uncertainty of earth system computer models is not just a challenge 126 for model developers but also for the users of the model outputs, such as 127 environmental managers and policy-makers. Inadequate description of the 128 uncertainties that affect model predictions may lead model users to 129 overestimate the model's predictive ability which might create the false belief that the model can adequately reproduce all the consequences of the decisions 130 131 to be made. On the other hand, ineffective communication of those 132 uncertainties may induce decision-makers to underestimate the model's 133 predictive ability and lead to rejecting the model predictions completely (Saltelli 134 and Funtowicz, 2013).

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136 The discussion so far highlights the importance of investigating uncertainty 137 propagation in computer models in earth system science for both scientific and operational purposes. This task is often performed by rather simple approaches 138 139 where uncertain input factors (such as input (forcing) data, model parameters 140 or even underlying assumptions) are changed one-at-a-time and the effect in 141 model predictions is assessed either visually or through simple quantitative 142 indicators such as "the amount of change in model predictions for a fixed variation of the investigated input". However, this approach quickly becomes 143 144 cumbersome if one has to investigate a large number of uncertain input factors.

145 It also does not guarantee to provide a full picture of the model's behaviour 146 given that only a limited number of input variations can be tested manually. 147 Therefore, there is an increasing agreement that more structured, transparent 148 and comprehensive approaches should be used to fully explore the impacts of 149 input uncertainties on computer model predictions. Global Sensitivity Analysis 150 (GSA) is a set of statistical analysis techniques that provides such a structured 151 approach (Saltelli et al., 2008). GSA can address questions like:

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 Which variable (or component) of a computer model mostly influences model predictions, when and where? Hence, is the model's behaviour consistent with our conceptual understanding of the system functioning?

- Which uncertain input (or assumption) mostly contributes to the uncertainty in the model predictions? Hence, where should we focus efforts for uncertainty reduction?
- Can we find thresholds in the input factor values that map into specific output regions (e.g. exceeding a stakeholder-relevant threshold) of particular interest? Hence, what are the tipping points that, if crossed, would bring the system to specific conditions we want to avoid or want to reach?
- How robust are model predictions to modelling assumptions? Hence,
 how much would model-informed decisions change if different
 assumptions were made?
- 166

167 GSA has the potential to massively advance the value of computer models in 168 the earth system sciences, contributing to improved model development, better 169 evaluation and more robust decision-making. However, despite such potential, 170 the application of GSA in many areas of earth system sciences is still relatively 171 limited. A recent literature survey by Ferretti et al. (2016) showed an increase 172 in the share of scientific articles using the term 'sensitivity analysis' (SA) since 173 the year 2004. They also found that the largest fraction of those papers uses a 174 'local' approach, whose differences with respect to the 'global' approach, on 175 which this paper focuses, will be clarified in the next section. We therefore 176 believe that there is a lot of potential to further expand the use of GSA and 177 benefit from its strengths.

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179 The goal of this paper is to demonstrate the value of GSA for the construction, 180 evaluation and use of earth system models by showing examples of what its 181 application has achieved so far for scientists, modellers and policy-makers. We 182 do not cover in-depth mathematical aspects of GSA algorithms, which the 183 interested reader may find in other recent reviews, e.g. Norton (2015) and 184 Pianosi et al. (2016). Also, differently from recent special issues and books on 185 GSA applications to earth system models and observations (e.g. Kettner and 186 Syvitski (2016) and Petropoulos and Srivastava (2017)), which focus on 187 individual methodological advances and novel applications of GSA, our aim is to provide a synthesis of some key and generic lessons that the earth science 188 189 community has learnt through the application of GSA over the last 15 years. 190 Through such review we hope to increase the appreciation of the approach in 191 a wider community and promote its uptake by a larger number of earth system 192 scientists.

194 In the next Section we introduce key definitions and concepts that are needed to understand the basic functioning of GSA and organise them into key 195 guidelines for GSA application. Then, we present several examples from the 196 197 literature where GSA was used to address the issues discussed in the 198 Introduction section on the topics of construction, evaluation and use of 199 computer models for earth sciences. Again, we organise this literature review 200 into 10 generic lessons learnt through the application of GSA to earth system models. We conclude our paper with what we think is an "A-B-C-D" for future 201 202 research and applications of GSA.

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204 2. A brief Introduction to GSA205

206 In this section, we discuss the basics of Sensitivity Analysis (SA) in general and 207 Global Sensitivity Analysis (GSA) in particular. We also provide key guidelines 208 for the application of GSA to earth system models. We use the term 'model' to 209 refer to a numerical procedure that aims at reproducing the behaviour of earth 210 system components, typically via numerical integration of differential equations 211 over a space and time domain. Because we assume such a numerical 212 procedure to be implemented by a computer algorithm, we could equally use 213 the term 'computer model' in this context. We further call 'input factor' any 214 element that can be changed before running the model, and 'output' any 215 variable that is obtained after the model's execution.

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Figure 2(a) provides examples of input factors. They can be broadly divided into four groups:

[1] The equations implemented in the model to represent physical processes,
for which our often-incomplete scientific knowledge might offer multiple options
(including omissions, if a process is deemed negligible given the scope and
scale of the application).

[2] Set-up choices that are needed for the execution of the model on a computer, for example the selection of temporal or spatial resolutions for numerical integration of the model equations.

[3] The numerical values to be attributed to the parameters appearing in the model equation, which are often 'effective' parameters i.e. quantities that cannot directly be measured due to a scale mismatch between model element and instrument footprint (Beven, 2002). These parameters are called 'effective' since they are typically set to values that make the model component, e.g. a soil moisture store, approximate the behaviour of the real-world system without representing the full heterogeneity of that system (Wagener and Gupta, 2005).

233 [4] Any input data (system forcing, initial conditions and boundary conditions), 234 which may be uncertain due to errors in both measurement and pre-processing 235 (Figure 2(b)). Examples of pre-processing errors include the spatial 236 interpolation of point observations or the manipulation of raw observations 237 (such as remote sensing data) to transform them into the actual variable 238 needed as input to the computer model. The importance of initial and boundary 239 conditions varies significantly with the type of model, for example the simulation 240 results of an atmospheric model might be very sensitive to uncertainty in initial

conditions, while those of a groundwater model will depend more strongly on
the assumed boundary conditions. The impact of initial conditions will also grow
over the simulation period for some models, e.g. numerical weather prediction
models, while it will diminish with time for others, such as rainfall-runoff models,
which means it might be less relevant if a sufficiently long warm-up period is
available in such cases.

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248 The specific goal of SA is to investigate the relative influence that input factors 249 have on one or more model outputs. If the relationship between input factors 250 and output is nonlinear, then small variations of an input factor (e.g. x_i) may 251 induce large variations in the output (y), while large variations of another input 252 factor (x_i) may induce much lower variations in the output. In such cases we 253 would say that x_i is more influential than x_i , or equivalently that y is more 254 sensitive to x_i than to x_j . Sometimes, output sensitivities can be estimated by 255 analysing the model equations directly (algebraic SA). However, when the 256 relationships between input factors and outputs are numerous and complex, 257 sensitivities can only be discovered 'empirically', i.e. by running the model 258 against different combinations (samples) of the input factors and by analysing 259 the statistical properties of the input-output sample (sampling-based SA). Since 260 algebraic SA is rarely a viable option in earth system models, in this paper we 261 focus on sampling-based SA and refer the reader to Norton (2008; 2015) for 262 algebraic SA.

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The following sections briefly outline and discuss key elements in any Global Sensitivity Analysis process. We focus mainly on the key choices a GSA user has to make in this process.

267268 2.1 Multiple definitions of the model output are possible

269 The model output y can be any variable that is obtained after model execution 270 and that is of interest for the user, for example the predicted value of the system 271 state at a prescribed time or location, or a summary metric such as the average 272 (or any other statistic) of time-varying and spatially-varying states (Figure 2(c)). 273 If observations of a simulated variable are available, the output y can also be 274 defined by an error metric that measures the distance between observed and 275 simulated variables, e.g. the mean squared error. In this case, what is called 276 'output' for the purposes of SA is not the 'output' of the computer model but 277 rather a measure of the model's predictive accuracy (or 'objective function' in 278 the automatic calibration literature).

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280 2.2 Global methods measure direct and joint effects of input factors 281 across their variability space (so no baseline point needs to be defined)

The simplest and most intuitive way to perform sampling-based SA is by a socalled 'One-At-a-Time' (OAT) approach. Here, baseline values for the input factors have to be defined and the input factors are varied, one at a time, by a prescribed amount (perturbation) while all others are held at baseline values. An example of OAT sampling for the case of 3 input factors is shown in Figure 3(a). SA results can be displayed for instance using a tornado plot (Figure 3(b)), which shows the output variations from the baseline, sorted from largest to smallest. If the perturbations applied to the baseline are small, the analysis is
referred to as *local* SA, and output sensitivities can be measured by the
(approximate) output derivatives at the baseline point.

- 293 The OAT approach is appealing as it calculates the variation in the model output 294 in relation to a baseline, which is easy to interpret if the baseline has a clear 295 meaning for the model user, for example the 'default' model set-up or the 296 'optimal' set-up after model calibration. Local methods are widely applied in 297 different fields of study - especially where the feasible number of model runs is 298 a limiting factor (Hill et al., 2016). However, the OAT approach has two main 299 disadvantages. Firstly, OAT sampling only explores a small portion of the space 300 of variability of the input factors, especially as the number of input factors 301 increases. Therefore, the OAT approach is mostly useful if one is interested in 302 exploring the model behaviour in relation to the baseline rather than across the 303 entire space of input variability. Secondly, the OAT approach cannot detect 304 interactions between input factors, i.e. the fact that the joint perturbations of two 305 (or more) input factors may induce larger (or smaller) output variations than the 306 perturbation of each individual factor. The latter problem can be partially 307 overcome in local SA, where second-order derivatives of the output can be 308 estimated with a relatively small number of additional model runs, thus 309 providing information about local interactions between input factors (see Norton 310 (2015) for more details). However, such sensitivity information is only valid in 311 the neighbourhood of the baseline point, which may be limiting if one needs to 312 investigate the effects of larger deviations or if there is simply no 'baseline' point 313 of particular interest.
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315 To address these issues and investigate the effects (direct and/or through 316 interactions) of input variations regardless of a baseline, 'global' approaches to 317 sensitivity analysis (GSA) have been proposed. In GSA, all input factors are 318 varied simultaneously with the objective of covering their joint variability space 319 as evenly as possible in accordance with the distributions underlying each 320 factor (Figure 3(c)). Different random sampling (e.g. Latin-Hypercube) or guasi-321 random sampling (e.g. Sobol') techniques can be applied to this end. The model 322 outputs obtained for all the sampled input factors can then be analysed 323 qualitatively (via visualisation techniques) and/or quantitatively (via statistical 324 techniques). Quantitative GSA methods typically provide a set of sensitivity 325 indices (Figure 3(d)), which measure the overall effects on the output from 326 varying each input factor, usually on a scale from 0 to 1. A simple practical 327 example of how to visualise and interpret a set of global sensitivity indices is 328 given in Figure 4. Examples of how global sensitivity indices can help overcome 329 the limitations of OAT approaches and avoid missing or misclassifying key 330 sensitivities are given for example by Saltelli and D'Hombres (2010) and Butler 331 et al. (2014).

332

333 2.3 Method choice matters as it can result in different sensitivity estimates 334 (so, using multiple methods is advisable)

335 Global sensitivity indices can be defined in several different ways. A review of 336 available methods is given for example by Pianosi et al. (2016) where a broad 337 classification was proposed comprising four classes: (1) multiple-start 338 perturbation approaches, where global sensitivity is obtained by aggregation of 339 'OAT' sensitivities obtained at different baseline points; (2) correlation and 340 regression approaches, where sensitivity is measured by the correlation 341 between input and output samples; (3) regional sensitivity analysis (or Monte 342 Carlo filtering) methods, where sensitivity is related to variations in the 343 distributions of input factors induced by conditioning the outputs; and (4) 344 variance-based and density-based approaches, where sensitivity is linked to 345 variations in the output distribution induced by conditioning the inputs. A more 346 in-depth discussion of these approaches and their advantages and 347 disadvantages goes beyond the scope of this review and can be found in Saltelli 348 et al. (2008), Pianosi et al. (2016) or Norton (2015).

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350 GSA methods are based on different assumptions and use different definitions 351 of sensitivity, which may lead to different sensitivity values and hence 352 differences in outcomes of ranking and screening of the input factors (e.g. Tang 353 et al. 2007a; Gan et al., 2014). A detailed discussion of this issue would be bevond the scope of this paper, but we generally suggest comparing the 354 355 outcomes of different methods to understand the impact of the assumptions 356 made. This multi-method approach can often be achieved very cheaply (in 357 computational terms) since the same input-output sample can be used to 358 estimate sensitivity indices according to different methods (e.g. Pianosi et al. 359 2017).

360

361 2.4 The definition of the space of variability of the input factors has 362 potentially a great impact on GSA results

363 Regardless of the GSA method chosen, a critical and yet not sufficiently 364 explored issue is the choice of the space of variability from which input factors 365 are sampled (i.e. the box in Figure 3c and the associated probability for 366 sampling). When the uncertain input factors are model parameters, sampling is 367 most often based on independent uniform distributions so that only the upper 368 and lower bounds for each parameter have to be defined. Yet this definition of 369 boundaries is often not easy to make, given the unclear physical meaning of 370 many of the parameters used in earth system models, i.e. their 'effective' nature 371 as discussed above. Some might vary from 0 to 1, and some might have at 372 least a fixed lower bound (usually 0), but often this is not the case. Several 373 papers (e.g. Kelleher et al., 2011; Shin et al., 2013; Wang et al., 2013) have 374 demonstrated that, when multiple choices for parameter ranges are acceptable, 375 changing the range for uniform sampling can significantly change the estimated 376 sensitivity indices. Paleari and Confalonieri (2016) analysed other parameter 377 distributions (e.g. normal) and found again that sensitivity estimates were 378 strongly affected by the chosen distribution parameters. So, a pitfall of GSA is 379 the possibly significant impact of the chosen input distributions, which should 380 be carefully scrutinised.

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Intuitively one might opt for relatively wide ranges to ensure that any impact of
a parameter is captured. However, this can lead to the problem that poorly
performing parameter values are included and impact the sensitivity analysis

(e.g. Kelleher et al., 2011). A key to understanding this problem is to combine 385 386 the GSA with an analysis of the performance of the simulations included in the 387 analysis so to possibly exclude poorly performing simulations and avoid that 388 they 'dominate' the estimation of sensitivity indices. Such a performance-based screening step would identify what is sometimes referred to as the behavioural 389 390 simulations, i.e. those that produce a performance metric above (or below) a 391 certain modeller chosen threshold value (Beven and Binley, 1992; Freer et 392 al., 1996). It is generally good advice to perform the sensitivity analysis with and without considering such performance screening to understand the potential 393 394 impact of poorly performing simulations on the sensitivity analysis result.

395

396 2.5 Sample size affects GSA results (so, the robustness of sensitivity 397 indices should be checked)

As intuitively understandable from Figure 3(c), GSA requires many more input 398 399 samples, and therefore more model executions, than OAT (local) SA. 400 Therefore, when the computing time for each model run is long and/or a large 401 memory space is required to store the output of each run, GSA can become 402 difficult to apply. While the number of model executions (*N*) typically increases 403 proportionally to the number of input factors (M), the proportionality relationship 404 between *M* and *N* can vary significantly from one method to another, as well as 405 from one application to another for the same method. As a rule of thumb, we 406 would say that the most frugal methods (e.g. multiple-starts perturbation 407 approaches) require around 10 to 100 model runs per uncertain input factor, 408 while more expensive methods (e.g. variance-based) may require a number as 409 large as 10,000 or even 100,000 times the number of input factors. This said, giving a 'one-fit-for-all' rule to link *M* to *N* can be misleading because it would 410 411 assume that all GSA applications with the same number of factors require the 412 same sample size, which is not the case (see for example Figure 5 in Pianosi 413 et al. (2016) and Sarrazin et al. (2016)).

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415 Given that the rules of thumb mentioned above can only provide very rough 416 guidance and the actual numbers can vary greatly with the model under study 417 (and even with the specific system to which the model is applied) we suggest 418 that, rather than worrying too much about the number of samples a priori, it is 419 better practice to analyse a posteriori the robustness of the GSA results. This 420 can for example be achieved via bootstrapping, a resampling strategy that 421 provides confidence limits on the sensitivity indices without the need for re-422 running the model (e.g. Sarrazin et al., 2016). Essentially, overlapping 423 confidence limits between factors suggest that no robust conclusion between 424 the importance of the factors can be drawn, and that the sample size should be 425 increased.

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Also, what sample size is adequate may vary depending on the GSA purpose.
In fact, while obtaining precise estimates of sensitivity indices (i.e. with narrow
confidence limits) may require a very large number of model executions,
several studies (e.g. the one discussed below by Baroni and Tarantola (2014)
and summarised in Fig. 5) have demonstrated that a robust separation between
influential and non-influential factors (referred to as 'screening' in the GSA

literature) or a robust ranking of the influential factors can often be obtained at
much lower sample size. Therefore, for these purposes, a relatively small
number of model executions is often sufficient even when applying a
supposedly expensive GSA method (Sarrazin et al., 2016).

438 Another critical issue arises when the objective of GSA is the screening of non-439 influential input factors. If sensitivity indices where calculated exactly, one 440 would simply test which factors have sensitivity indices of zero. However, 441 approximation errors generally mean that values will deviate from zero even for 442 non-influential factors. Additionally, users might also want to screen out factors 443 with very little influence on the model output. Typically, users subjectively select 444 a threshold to cope with this problem. Any factor showing a sensitivity index 445 value below this threshold is assumed to be non-influential (e.g. Van 446 Werkhoven et al., 2009; or Vanrolleghem et al., 2015 for an application and 447 methodology to set the screening threshold). Alternatively, Zadeh et al. (2017) 448 suggested the use of a dummy factor. This dummy factor is added to the model 449 in a way that its variability does not influence the model output by design. Therefore, the sensitivity index value obtained for this dummy factor is an 450 451 estimate of the approximation error only. Hence, it provides a threshold to 452 discriminate between factors that can be confidently considered influential, 453 since their sensitivity index exceeds this threshold, and those that may be non-454 influential, because they have an index around or below the threshold.

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Another option to reduce the computational burden of GSA is the use of an emulator, i.e. a computationally efficient algebraic representation of the original complex computer model, which is able to approximate the input-output relationship of the original model and can be used in its place during computationally expensive GSA applications (e.g. Borgonovo et al. 2012; Ratto et al., 2012; Girard et al., 2016; Verrelst et al., 2016).

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463 3. Review of GSA applications in earth system modelling and lessons 464 learnt

465 466 In this section, we present applications of GSA to earth system models or to 467 models of earth system components. We structure our review as 10 key lessons 468 learnt through application of GSA and their implications for the construction and 469 use of computer models in earth system sciences. These lessons cover 470 different stages of the model building and application process, from model 471 calibration (lessons 1,2,3,4), to the assessment and improvement of the data 472 used to force or calibrate the model (4,5,6), model evaluation/validation (2,7,8) and the use of models in support of decision-making (9,10). We use examples 473 from a variety of earth science disciplines although some disciplines are 474 475 relatively more represented because the use of GSA in those areas is more 476 widespread. One example of such an area is hydrology as is visible from the 477 extensive review by Xiaomeng et al. (2015).

3.1 Only a small number of parameters typically dominates the variability of a given model output, though which parameters are dominant might vary with the chosen error or summary metric

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A key observation when performing GSA to measure the relative importance of uncertain parameters is that the number of parameters that control the variability of a specific model output, be it defined as a summary or error metric, is rather low, typically in the order of 5 or 6 parameters. Other parameters might have a small direct effect or be involved through interactions, but they are not dominant.

489 An example is given in the top panel of Figure 5 where Wang et al. (2013) showed that out of 47 parameters of a crop growth model, less than 10 have a 490 491 dominant influence on the selected output (final yield). Other examples with 492 similar conclusions include Ben Touhami et al. (2013) for an ecological model, 493 Girard et al (2016) for an atmospheric dispersion model; Bastidas et al. (1999) 494 for a land surface model, Esmaeili et al. (2014) for a water quality model, and 495 many others for hydrological models (e.g. Wagener et al., 2001; Van Werkhoven et al., 2009; Massmann and Holzmann, 2015; Hartmann et al., 496 497 2017; Shin and Kim, 2017).

498 The main implication of this limited number of influential parameters is that, if a 499 computer model is mainly used to predict a specific summary metric (like annual yield as discussed in the previous paragraph), or it needs to be calibrated 500 501 according to a given error metric (like the Root Mean Squared Error), it is often 502 possible to significantly reduce the cost of model calibration (e.g. acquisition of 503 new data to constrain the parameter values, or use of computationally-504 expensive automatic calibration algorithms to determine 'optimal' parameter estimates) by focusing on the small subset of parameters that are influential for 505 506 that metric. The non-influential parameters can simply be set to 'default' values 507 (taken from literature or previous applications) without significantly affecting 508 model predictions or their accuracy.

509 On the other hand, this also means that there is an opportunity to define multiple 510 output metrics (for example high and low river flows in hydrologic models), 511 which are controlled by different parameters, to identify all or at least most of 512 the model parameters. And indeed, GSA examples where multiple outputs 513 were used, consistently demonstrated that different outputs are sensitive to 514 different subsets of parameters (e.g. Bastidas et al., 1999; Tang et al., 2007a; 515 Rosolem et al., 2012; Gan et al., 2015). An example is given in the bottom panel 516 of Figure 5, taken from Song et al. (2012). Importantly for our argument here, 517 the influential parameters vary somewhat across outputs but the total number 518 per output remains small. A consequence of this finding is that if we want to 519 understand the level of model complexity that is supported by a given dataset, 520 we must take great care in defining several contrasting output metrics to 521 maximize our chances of extracting all relevant information from the data (e.g. 522 Gupta et al., 2008).

523 **3.2 Dominant parameters can vary with the earth system (location)** 524 **modelled**

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526 Besides varying with the output metric chosen by the modeller, parameter 527 sensitivities can also vary when the same computer model is applied to different 528 earth system locations (e.g. different catchments or drainage basins). We 529 typically assume that our models have a degree of generality, i.e. that they are 530 not only build to represent a single system, such as a particular catchment or 531 hillslope, but that they can be used to represent the behaviour of the same type 532 of system at different locations. A single model is then tailored to different 533 locations when its model parameters are assigned values to reflect the specific 534 characteristics of the system under study.

535 For example, Rosero et al. (2010) analysed a land surface model across different meteorological monitoring sites in the southern USA. The sites are 536 537 located along a precipitation gradient and they also differ in land use and soil 538 types. The assumption in their study was that the vegetation and soil 539 parameters of the physically-based land surface model would be controlled by 540 the differences in land use and soil type. However, they found that the dominant 541 control on these parameters was the variability in precipitation, thus putting the 542 physical interpretation of the parameters into question and suggesting that they 543 are effective parameters. The importance of climate characteristics in 544 conditioning parameter behaviour is further demonstrated in Van Werkhoven et 545 al. (2008a). Here, parameter sensitivities for a conceptual rainfall-runoff model 546 were computed in 12 catchments located in increasingly drier climates. The 547 results (shown in Figure 6) revealed that parameter sensitivity varies with the 548 output metric and application site, and that some of this variability can be linked 549 to climatic characteristics, since patterns of increasing or decreasing sensitivity 550 are found when moving from drier to wetter catchments. Other GSA 551 applications showing similar variability of parameter sensitivities with the 552 model's application locations include Confalonieri et al. (2010); Ben Touhami 553 et al. (2013), Shin et al. (2013), Hartmann et al. (2013) and Herman et al. 554 (2013).

555 A practical implication of this finding is that when calibrating a computer model 556 for a new site, one should avoid making assumptions based on extrapolation 557 from GSA results obtained elsewhere. For the purpose of better understanding 558 the model behaviour, it is also interesting to investigate how parameter 559 sensitivities vary from site to site and to test whether these variations can be 560 linked to the site's physical or climatic characteristics. This could be reasonably 561 expected when parameters are assumed to correspond to physical 562 characteristics of the modelled system. Application of formal GSA may confirm 563 or challenge this expectation.

564 **3.3 Parameter sensitivity often varies in space (across the simulation** 565 **domain) and in time (over the simulation period)**

So far, we discussed GSA applications where the model output y is a scalar 567 568 variable obtained by aggregation of the temporally and/or spatially distributed 569 predictions of the model - either as an aggregation of the model outputs or state variables, or as an error metric derived from the difference between 570 571 simulated and observed outputs (see Fig. 2c). In both cases, it is likely that this 572 aggregation leads to a loss of information in both space and time. For example, 573 when calibrating a rainfall-runoff model we normally estimate any measure of 574 model performance (i.e. an error metric) over a sufficiently long and variable 575 time period to trigger a range of responses of the model (Yapo et al., 1999). 576 This maximises our chances of extracting sufficient information from the data 577 to calibrate the parameters of interest. Conversely, the temporal aggregation 578 does not reveal when in time each parameter is controlling the model's 579 response and when it is not.

580

581 However, we can avoid this information loss by estimating disaggregated 582 sensitivity indices in space and time. Applications of GSA where the analysis is 583 applied to either individual time steps or to a small moving window period have 584 become common. One interesting application of such time varving sensitivity 585 analysis is a comparison between active model controls and expected process 586 controls during different response modes of the system (e.g. Wagener et al., 587 2003; Reusser et al., 2011; Vezzaro and Mikkelsen, 2012; Guse et al., 2014; 588 Pfannerstill et al., 2015). We will discuss this time varying analysis of parameter 589 sensitivity in detail in section 3.7 in the context of model validation.

590

591 An example of spatial GSA results, focused on understanding how sensitivity 592 indices vary across a model's domain, is given in Figure 7 for a computer model 593 of chemical transport in the atmosphere. In this study, Brewer et al. (2017) 594 showed that parameter sensitivities can exhibit complex spatial patterns, with 595 some parameters being very influential but only in specific portions of the 596 simulated spatial domain. These insights are very useful to tailor the model 597 calibration efforts to where it is most effective, a piece of information that would 598 otherwise be lost if applying GSA to aggregate output metrics. High levels of 599 spatial variability in parameter sensitivities were also reported in Sieber and Uhlenbrook (2005), Hall et al. (2005), Treml et al. (2015), and in Savage et al. 600 (2017). Tang et al. (2007b) and Van Werkhoven et al. (2008b) additionally 601 602 linked the spatial variability of sensitivity indices to the spatial variability of 603 forcing inputs.

604

605 Avoiding the loss of information induced by using aggregate output metrics has 606 consequences for a range of activities, including model calibration, model 607 validation and evaluation, observation network design etc. GSA can be used to understand which data periods or which domain parts contain information and 608 609 which do not. Such analyses also highlight opportunities for creating more 610 detailed models without adding parameters that cannot be identified. We 611 provide further examples of the value of disaggregation in sections 3.7 and 3.8. 612

613 3.4 Uncertainty in the observations of the system outputs can prove as 614 influential as uncertainty in the model parameters or forcing inputs

616 A big challenge in earth systems modelling is that the observations of the 617 variables simulated by the computer model are often affected by large errors. 618 If error metrics are very sensitive to such errors, their value for evaluating model 619 accuracy and guiding model calibration is undermined. GSA can be used to 620 explore the issue in a formal way by including errors in observations among the 621 uncertain input factors subject to the sensitivity analysis (several techniques to 622 do this are discussed in Sec. 4.3.2 of Pianosi et al. (2016)) and can be used to 623 quantify their relative influence with respect to uncertain parameters or other 624 factors.

625

626 Figure 8 depicts an example for a computer model of soil-water-atmosphere-627 plant dynamics by Baroni and Tarantola (2014). Here, uncertainty in soil 628 moisture observations was found to influence model accuracy (measured using 629 the root mean squared error between simulated and observed soil moisture) as 630 much as uncertainty in the soil parameters. Moreover, the analysis showed a 631 high level of interactions between the two uncertain factors, which implies that 632 parameters can only be properly estimated if the uncertainty in the soil moisture 633 observations is simultaneously reduced.

634

635 Uncertainty in the observations of the system outputs are regularly ignored in 636 modelling studies once an error metric (which typically encapsulates a set of 637 assumptions about the statistical properties of the observational errors) has 638 been defined. Observations of system outputs are the main data that we 639 evaluate our model against, both when estimating parameters (calibration) and 640 when making predictions (what is sometimes called 'validation'). However, the 641 potentially large uncertainties in such observations are increasingly recognised 642 (see for example Westerberg and McMillan (2015) or Coxon et al. (2005) for an assessment of uncertainty in streamflow observations). We still require a better 643 644 understanding of the implications of such uncertainties, especially when it 645 comes to predictions of extremes (such as floods or heatwaves) for which 646 observations are sparser and more error prone. This is an under-researched 647 area in terms of GSA applications and where GSA has the potential to help us 648 learn much about how influential such uncertainties can be.

649

3.5 Uncertainty in forcing input data affects model output uncertainty, not only because of errors in the measurements but also because of uncertainties in data pre-processing

653

654 Similarly to considering uncertainty in observations of the system output, GSA 655 can also be used to analyse the impact of uncertainty in the input data of the model simulation, such as forcing data and initial or boundary conditions. For 656 657 example, in the GSA application presented in Figure 8 (Baroni and Tarantola, 658 2014), errors in the time series of weather forcing data (air temperature, 659 humidity, wind, rain and global radiation) were included in the analysis, 660 although in this particular case they proved to have a relatively negligible effect 661 on the model output. The result is case specific and other GSA applications 662 found that uncertainty in the such inputs can at times be as influential as

663 parameter uncertainty (e.g. Pianosi and Wagener (2016)). Figure 9 shows another interesting example taken from Yatheendradas et al. (2008) for a 664 665 distributed hydrological model. Here, the forcing input was based on rainfall estimates from radar reflectivity measurements. The GSA showed that the 666 uncertainty in the parameters translating the reflectivity signal into rainfall 667 668 estimates (the so-called Z-R relationship) dominated the uncertainty in the flow 669 predictions and was more influential than the uncertainty in the parameters or 670 initial conditions of the hydrological model. Hence there is little to be gained by 671 improving the hydrological model unless this pre-processing uncertainty can 672 first be reduced.

673

674 This is a nice example of the difficulty in distinguishing between errors in the 675 'main' hypothesis, i.e. the earth system computer model, and in the 'auxiliary' hypothesis, i.e. the pre-processing procedure by which the model forcing inputs 676 677 are generated (Oreskes et al., 1994). The latter is subject to uncertain 678 assumptions that may prove as important as those embedded in the model. A 679 typical problem in this context is that there is often little additional information 680 available to determine such uncertainties (e.g. discussion in Beven and Cloke 681 (2012)), which are therefore poorly understood. Approaches to back-out the 682 uncertainty in the forcing data through inverse analysis of hydrological models 683 have shown that the result depends strongly on other assumptions made 684 (Renard et al., 2010; 2011). It is therefore important to understand the potential 685 impact and relevance of such data pre-processing uncertainties so that efforts 686 to reduce the final model output uncertainty can be pointed to the right factors 687 (forcing data, parameters, output observations, etc).

688

689 3.6 Discrete modelling choices can be as influential as the uncertainty in 690 parameters or in data

691

692 A common issue in earth system modelling is that model developers have to 693 make discrete modelling choices or uncertain assumptions, for instance about 694 which equation should be used to represent a specific process, or about the 695 appropriate temporal or spatial resolution for the numerical integration of 696 differential equations. One might therefore want to know how much these 697 modelling choices matter given uncertainties in the model parameters, in the 698 input data and in other elements of the modelling chain. Although much less 699 explored, GSA can be used to address this guestion because it can quantify 700 the relative influence of discrete modelling choices on model predictions. A 701 simple strategy to achieve this aim is to include among the uncertain input 702 factors x_i a discrete random variable that switches between a finite number of 703 possible values. Each of these values corresponds to one of the possible 704 discrete choices, so that the relative importance of that choice can be compared 705 to that of the other uncertain factors.

706

An example of how to implement this strategy is provided again in the hydrology field by Baroni and Tarantola (2014). In their study, the model's vertical resolution was included in the GSA and found to play a negligible role with respect to parameter and data uncertainty as can be seen in Figure 8. Savage 711 et al. (2017) instead found – using the same strategy – that the choice of the 712 spatial resolution grid can have a significant influence on flood inundation 713 predictions. It can even overtake the uncertainties in parameters and boundary 714 conditions, although the ranking of these uncertain input factors varies in time, 715 space and with the flood metric (output v) used. Another example, again for 716 flood prediction, is the study by Abily et al. (2016) shown in Figure 10. Here 717 GSA revealed that the chosen spatial resolution grid and the level of detail in 718 describing above ground features affected water depth predictions more than 719 errors in high-resolution topographic data.

720

721 The cited studies demonstrate that the importance of discrete modelling 722 choices can be quantified in a structured way just as traditionally done for 723 uncertainty sources such as parameters and forcing data. By doing so, the 724 authors show that these discrete choices can be as significant as the 725 continuous uncertainties more typically considered. By revealing when such 726 discrete choices (or uncertainties) matter relative to other uncertainty sources, 727 GSA provides a formal criterion to assess whether simplifying choices are 728 acceptable. The analysis might also help to prioritise efforts for model 729 improvement.

730

3.7 Consistency of model behaviour with the underlying perceptual model of the system is as important as the ability to reproduce observations

733

734 Another reason for using GSA is to evaluate the consistency between the model 735 behaviour and the modeller's expectations, i.e. their 'perceptual model' of the 736 system. GSA can contribute to this task by providing a formal assessment of 737 the dominant controls on the model outputs, possibly disaggregated in space 738 and time. A minimum requirement for a computer model to be considered 739 acceptable is that these patterns of dominance are consistent with the 740 modeller's understanding of the system's dominant drivers. We would say this 741 criterion reflects Oreskes et al (1994) definition of model validation as 742 demonstration of the model's "internal consistency".

743

744 An example is given in Figure 11 for the case of a hydrological model from the study by Reusser and Zehe (2011). Here, different groups of parameters 745 746 represent different flow formation processes, which means they are expected 747 to be more or less influential as hydro-meteorological conditions vary. The 748 authors used time-varying GSA to quantify the temporal patterns of parameter 749 influence and to identify events where those patterns were not consistent with 750 expectations. Further scrutiny of simulated variables and sensitivities during 751 these events helped to identify weaknesses in the model, e.g. missing processes, and systematic errors in the data used to assess model predictions. 752 753 Other examples from hydrology include Wagener et al. (2003), Sieber and 754 Uhlenbrook (2005), Pfannerstill et al. (2015), or Kelleher et al. (2015). This type 755 of GSA utilization is also increasing in other areas of the earth system sciences, 756 recent examples being Treml et al. (2015) (larvae dispersal in the ocean) and 757 Arnaud et al. (2016) (soil-landscape evolution).

759 The conclusions of these studies are in line with the suggestion that consistency 760 with the underlying perception of the real-world system is equally or potentially 761 even more important than the optimal fit to available observations (Wagener 762 and Gupta, 2005). Moving beyond model fit-to-data as the main model quality 763 criterion, and rather focusing on the concept of consistency, has proven highly 764 beneficial in model assessment (Martinez and Gupta, 2011; Euser et al., 2013; 765 Hrachowitz et al., 2014; Pfannerstill et al., 2015; Shafii and Tolson, 2015). This 766 finding has wide reaching implications that have so far not been fully 767 appreciated, therefore leaving much room for further exploration. The current 768 predominant approach to model evaluation still largely relies on the comparison 769 of modelled and observed system outputs. In this traditional approach, a model 770 is proclaimed to have been 'validated' if predictions are reasonably close to 771 observations, particularly if the match is achieved on a sub-sample of the 772 available dataset that was not used during model calibration. However, such an 773 optimal fit of predictions to observations might be a relatively fragile result, as 774 discussed for example in Beven and Binley (1992) and many subsequent 775 papers by Beven. It is easy to unintentionally fit the noise in the data, which is 776 often poorly known, or to obtain biased parameter estimates because of 777 unaccounted for errors in either forcing inputs or output observations. Biased 778 parameters estimates can also be obtained because the calibration dataset is 779 small and/or not representative of the entire range of system conditions (a 780 typical example in hydrology being a dataset that predominantly includes 781 particularly dry or wet years). The bias can also be caused because any chosen 782 error metric is likely to only capture some aspects of the system response. A 783 typical example is the root mean squared error, which in a hydrological model 784 would be largely controlled by the model's ability to reproduce flow peaks and 785 less by its ability to reproduce other aspects of the hydrological system, such 786 as the volume error. The problem is even more relevant if the modelling 787 objective is hypothesis testing regarding dominant processes, or if the model is 788 expected to provide longer term projections with changing boundary (e.g. 789 climate) or system (e.g. land use) conditions (Fowler et al., 2016). Here 790 understanding how the model represents system controls, and how such 791 controls in the model might change in the future, is crucial and much more 792 important than the model's ability to reproduce historical observations.

793

3.8 The design of observation networks and measurement campaigns can be more effective when analysing how the data information content varies in space and time

797

A question regularly encountered in earth system sciences is when and/or where measurements should be taken in order to maximize uncertainty reduction in model parameters, input forcing data, and ultimately model predictions. Cost-effective data collection requires a good understanding about which measurements are informative so that a targeted field campaign or an observational network can be designed (Moss, 1979).

804

An example is Raleigh et al. (2015), who used GSA to explore how different error characteristics (e.g. type, magnitude and distribution) in different forcing 807 inputs (such as air temperature, precipitation, wind speed, etc.) influenced 808 predicted snow variables such as snow water equivalent and ablation rates. 809 Another example is provided by Wang et al. (2017), who analysed when isotope 810 samples from streams should be collected to reduce the uncertainty in model 811 parameters. Using time-varying GSA, they showed that specific time periods 812 provide more informative samples for different parameters. Furthermore, they 813 demonstrated that taking only 2 samples during the appropriate hydrologic 814 conditions was as effective for uncertainty reduction as using all the 100 815 available samples from the entire data collection period. A slightly more 816 complex issue is where to take measurements across a spatial domain. An 817 example where GSA is used to answer this question is described in van 818 Werkhoven et al. (2008b) (discussed in detail in section 3.3). Here, spatially-819 varying sensitivities of a distributed hydrologic model revealed that at least one 820 more streamflow gauging station was required in the catchment to ensure 821 identifiability of the model parameters.

- 823 We believe that this issue is one of the most interesting application areas for 824 GSA in the years to come. Growing model complexity, dramatically increasing 825 data volumes and novel sensors continually change the problem of which data 826 are required for model identification and hypothesis testing. Addressing this 827 problem demands powerful frameworks for the optimal design of measurement 828 campaigns. Advances in modelling and sensing techniques also offer new 829 interesting questions for GSA. For example, can we achieve a similar 830 uncertainty reduction by applying many mobile and often much cheaper 831 sensors over a short time period compared to what is achieved by a much more 832 expensive continuous measurement station? Surprisingly though, this has so 833 far been one of the less active areas of GSA studies.
- 834

822

3.9 If model predictions are expected to support decision-making, then they have to be sensitive to decision-related input factors

837 As discussed in the Introduction section, earth system models are increasingly 838 used as tools to support decision-making, often in combination with socioeconomic models. In this case, input factors of a single or of several models 839 840 are related to possible planning/management decisions (for example, a model's 841 input factor may define the land use practices in agricultural areas, or the 842 operating rules for managing a reservoir, or do we have to evacuate an area 843 due to a high probability of flooding). The model is then used to assess and 844 compare the effects of different decisions (input factors) on an output of interest 845 (for example, a drought index or the biomass produced in a growing season). In this context, GSA can be used to quantify the effects of decision-related input 846 847 factors in the context of other uncertain factors (such as the parameters or 848 forcing inputs of the earth system model) that also influence the output of 849 interest but are outside the decision-maker's control. In fact, one would hope 850 that the decision-related input factors exert an influence on the output that is at 851 least comparable to that of other factors - otherwise the decision-making problem would be ill-posed. While this influence might be present in the real 852 world, one cannot take for granted that it also happens in the computer model 853

that is used to reproduce this reality. Indeed, models built for supporting decision-making typically integrate a range of interacting and often nonlinear components, which means that their responses to variations across their many input factors are not immediately obvious.

858

859 Examples of GSA applications to assess the relative influence of decision-860 relevant inputs include the study by Pastres et al. (1999), who applied GSA to 861 a model of the Venice lagoon to estimate the relative importance of controllable 862 drivers (e.g. nitrogen load or reaeration rate) and uncontrollable ones (e.g. 863 dispersion coefficients or initial algae density) on anoxic crises. GSA results 864 showed that variability in the initial algae density dominates the predicted 865 duration of anoxic conditions, while the reaeration rate and the nitrogen load 866 play a minor role. For management purposes this implies that measures aimed 867 at short-term reduction of nitrogen loading may not be effective if not combined 868 with long-term actions to reduce the accumulation of algae. Another example is the study by Xie et al. (2017), who used time-varying GSA of a hydrologic 869 870 and sediment transport model to identify the dominant drivers of sediment 871 export in the Three Gorge reservoir region and hence prioritise land 872 management practices.

873

While models are indisputably irreplaceable and useful components of many decision-making processes, GSA can sometimes reveal that specific models are ineffective in their role. Several studies have used GSA to assess the robustness of model-informed decisions to the uncertain assumptions and choices made throughout the modelling exercise, which typically include both natural and socio-economic components.

880

881 A famous example is given by Saltelli and D'Hombres (2010), who used GSA 882 to re-analyse the results of the Stern review (Stern et al., 2006) of economic 883 impacts due to climate change. They found that predicted GDP losses varied 884 dramatically with the assumptions made regarding both socio-economic factors 885 (e.g. discount rate) and physical factors (e.g. climate response to GHG 886 emissions), which implies that any inference drawn from such quantitative predictions would be very fragile. Another example of GSA of an integrated 887 888 assessment model is given by Butler et al. (2014). Here the authors found that 889 decision-relevant output metrics such as climate damage and abatement costs 890 were largely insensitive to climate-related parameters (e.g. land use change, 891 non-CO2 greenhouse gases, the carbon cycle model, and the climate model) 892 because they were largely controlled by the uncertainty in economic 893 parameters (e.g. the discount rate). The implication is that the performance of 894 different simulated policy options is more strongly controlled by the socioeconomic assumptions embedded in the model, than by their policy 895 896 characteristics - in other words, the model predictions tell us more about the 897 consequences of the assumptions made than they tell us about the different 898 policy options. A third example is given by Le Cozannet et al. (2015), who used 899 a time-varying GSA to determine the factors that mostly controlled the 900 vulnerability of coastal flood defences over time (Figure 12). They found that -901 for their question – global climate change scenarios only matter for long-term planning while local factors such as near-shore coastal bathymetry – whose
uncertainty is often neglected in impact studies – dominated in the short and
mid-term (say over the next 50 years).

905

906 These studies demonstrate the importance of understanding the dominant 907 controls of a model, in the context of the uncertainties that affects it, before the 908 model can be used for impact assessment. It is crucial to understand the actual 909 ability of a model to discriminate between decision options to avoid 910 unreasonably conditioning the impact assessment results on the modelling 911 choices made. While we assume that decision support models are generally build with the best of intentions, it is important to provide the evidence that the 912 913 intentions have been achieved.

914

3.10 Even in the presence of practically unbounded uncertainties, learning about the relationship between model controls and outputs can be relevant for decision-making

918 Another area where GSA has been successfully employed is the investigation 919 of so called 'deep uncertainties' (e.g. Bankes, 2002), i.e. input factors whose 920 ranges of variability and probability distributions are poorly known and hence 921 practically unbounded. A typical example are future carbon emission scenarios, 922 which can diverge massively and whose probability of occurring is totally 923 unknown.

924

925 The propagation of practically unbounded uncertain input factors through a model is technically feasible - it will be sufficient to consider all possible input 926 927 values or sample from very wide ranges. However, the resulting model 928 predictions are typically spread over such wide ranges that they are hardly 929 usable to directly inform decision makers. Approaches that assess the risk and 930 consequences of selecting a particular policy have been advocated as a more useful alternative strategy (Lempert et al., 2004). In these approaches, 931 932 decision-relevant insights are extracted from the model simulations by adopting 933 a so called 'bottom-up' (e.g. Wilby and Dessai (2010)) or 'scenario-discovery' 934 strategy (Bryant and Lempert (2010)), which in turn can be implemented 935 through a 'factor mapping' GSA technique. The idea is to start by defining 936 thresholds (e.g. extreme values) for output variables that are relevant for 937 decision-making, for example because exceeding the threshold is undesirable 938 and would require taking actions. One can then create a large number of 939 possible scenarios (e.g. of future climate) that are propagated through the 940 model and for which the appropriate output variables are calculated. GSA can 941 then be used to analyse these set of simulations and identify thresholds in the 942 input factors that, if exceeded, would cause the output to cross the undesired 943 thresholds. Decision-makers can further complement these results with other 944 sources of information to assess how likely those input thresholds are to be 945 crossed in the future and hence determine whether actions may be required.

946

947 Applications of this approach have been particularly reported for planning and948 management of water resource systems, some examples being Brown et al.

949 (2012), Kasprzyk et al. (2013), Singh et al. (2014) and Herman and Giuliani 950 (2018). Figure 13 instead reports an example for landslide risk assessment 951 taken from Almeida et al. (2017). Here the authors analysed the dominant 952 controls of a rainfall-triggered mechanistic landslide model and found that 953 uncertainty related to some physical slope properties can be as important as 954 deep uncertainties related to future changes in rainfall in determining landslide 955 occurrence (Figure 13).

956

957 The use of GSA for mapping of potentially very large and complex input-output 958 datasets offers great potential for detailed analyses, especially in the context of highly uncertain decision-making problems. Maybe surprisingly, powerful GSA 959 960 algorithms for mapping are not yet available, especially for situations where 961 strong interactions between input factors exist, and most of the factor mapping 962 applications mainly rely on visual tools more than quantitative approaches. This 963 problem offers a lot of opportunity for research advancements. One very appealing feature of this strategy is that it requires the definition of vulnerability 964 965 regions in the output space (e.g. what are critical thresholds such as the bankfull discharge in flood modelling). Defining this vulnerability space is often 966 967 only possible for the stakeholder or the decision maker, which therefore offers 968 communication opportunities between them and the modeller.

969

970 **Outlook** 971

972 Global Sensitivity Analysis (GSA) has become a widely-applied tool to 973 understand earth system models across processes, scales and places. Our 974 intention in this review paper was to organize and share some of the findings 975 that have been made using GSA across earth system model applications. We 976 believe that understanding what we have learned so far, and how these insights 977 have been obtained, is key to guide further model development and to achieve 978 robust decision-making using earth system model predictions. To this end, 979 instead of attempting a comprehensive review of a large number of papers, we 980 selected examples that we found particularly informative and accessible and 981 discussed them in some depth. We tried as much as possible to provide 982 additional references of other examples on the same issue (preferably in other 983 earth system domains) as opportunity for further reading and study.

984

In addition to these findings, we also attempt here to identify some common
characteristics in the way GSA was implemented in the most insightful
applications. We call this an "ABCD" for maximising the scientific insights
produced by GSA. It contains the following considerations:

989

A – Adaptability of the model to different environmental conditions changes the
 relevance of its input factors. It is therefore important to compare GSA results
 across a representative range of environmental conditions, including different
 places and different time periods.

994

B – Behavioural input factor samples might produce quite different sensitivity
 estimates compared to the samples taken from the full factor space. One should

997 consider whether very poor performing input factor combinations are998 conditioning the GSA results.

999

1000 C - *Combining* different SA methods, especially visual and quantitative ones,
1001 increases insight and robustness of the analysis. Using a single GSA approach,
1002 with its specific assumptions, might provide a skewed picture of the actual
1003 model behaviour.

1004

D – *Disaggregating* inputs and outputs in both space and time increases the amount of information extracted during the analysis. A very simple, but also very effective way, to enhance learning during GSA studies is to estimate sensitivity indices for sub-periods or sub-domains.

1009

1010 Much, if not all, of earth system science relies on the use of models. Even if we 1011 do not use a computer model to simulate or forecast the system response, we 1012 are still likely to use a model of sorts to translate raw observations (e.g. from a 1013 remote sensing) into a variable of interest (e.g. soil moisture). Understanding 1014 how these models' function is crucial for robust science. The complexity of 1015 these models quickly outruns our ability to analyse their behaviour without 1016 formal approaches to do so. Computational science has in recent years been 1017 challenged to ensure that its studies and their outcomes are reproducible. 1018 transparent and robust (Peng, 2011; Hutton et al., 2016). This challenge is 1019 growing guickly in size with the continuing increase in model complexity which 1020 can make GSA problematic due to computational constraints. Nonetheless, we 1021 believe that GSA offers an important way to respond to this challenge and our 1022 review hopefully provides examples of how effective GSA can be in this regard.

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1023

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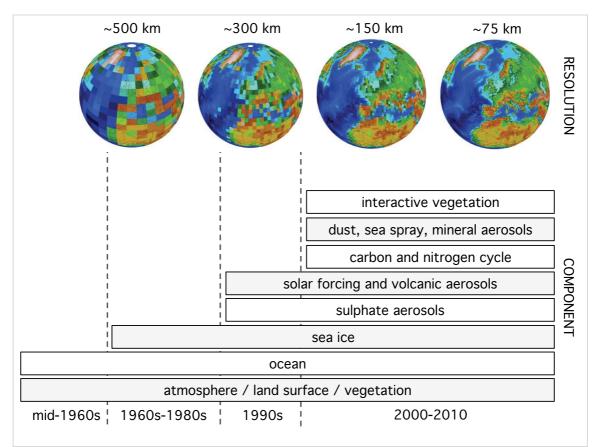


Figure 1. Increase in complexity of earth system models made possible by growing computing power: an example from atmospheric and ocean climate models. Top: growth in spatial resolution, bottom: growth in number of model components. Authors' elaboration based on Washington et al. (2012).

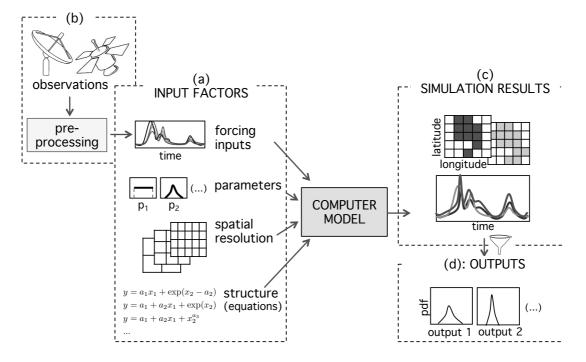


Figure 2. Schematic illustrating the (uncertain) 'input factors' and 'outputs' of a computer model, whose relationships are investigated by GSA.



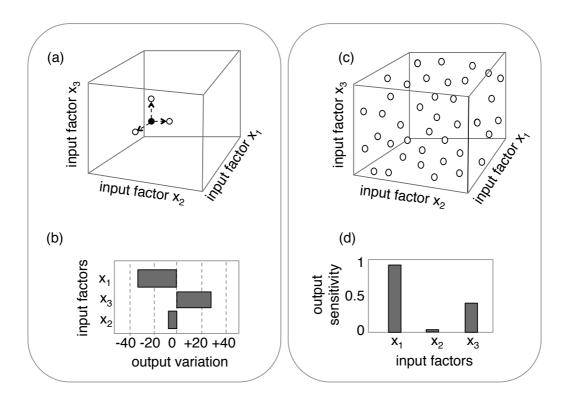


Figure 3. Schematic illustrating the difference between One-At-the-Time (OAT) sampling (a) and associated SA results (b) against All-At-the-Time (simultaneous) sampling (c) and corresponding sensitivity indices (d).

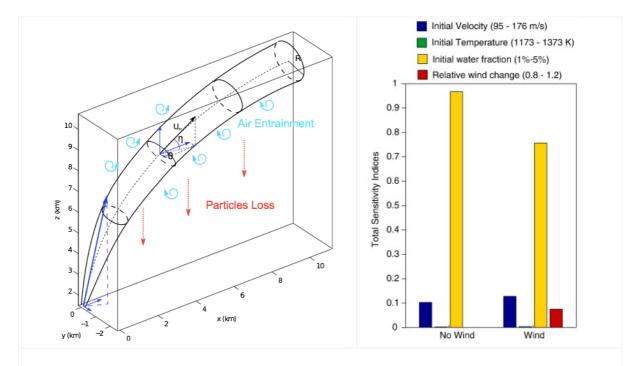


Figure 4. An example of GSA results for investigating the relative influence of four parameters on volcanic plume height predictions. Left: a schematic of the volcanic plume computer model taken from de' Michieli Vitturi et al. (2015). The model output *y* is the plume height attained at the end of the simulation period. Right: sensitivity indices (from de' Michieli Vitturi et al. (2016)) when varying the parameters in the ranges specified in the legend and under two weather scenarios ("wind" or "no wind" conditions). In both scenarios, the initial water fraction is associated with the largest sensitivity index, which means that that varying this parameter has the greatest influence on predicted plume height. Initial velocity is the second most influential input. Relative wind change has an influence only when wind is taken into account (as reasonable), and initial temperature has no influence given that the sensitivity index is close to zero in both scenarios. These results are useful for assessing the consistency of the model's behaviour and to prioritise the variables that would require targeted research in order to have the greatest reduction in output uncertainty.



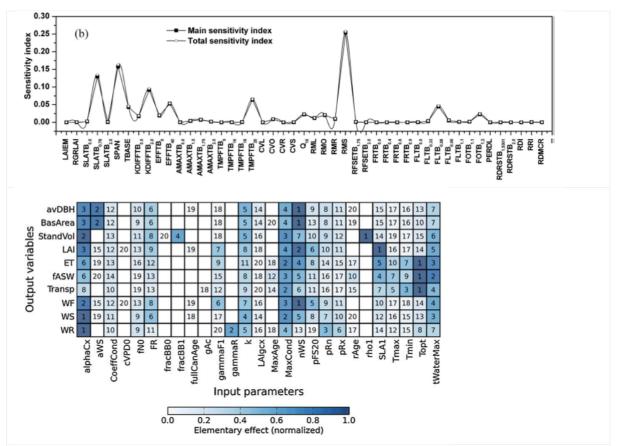


Figure 5. Examples of using GSA to analyse the relative influence of parameters on model predictions. Top: sensitivity indices of the 48 parameters of a crop growth model (taken from Wang et al., 2013). Most of the parameters have a sensitivity index close to zero, meaning that their influence on the selected output metric (the simulated final yield) is negligible. Bottom: sensitivity indices of the 27 parameters of a forest growth model for 10 different output metrics, each representing a different aspect of simulated biomass growth and water exchange between soil, plants and atmosphere (taken from Song et al. 2012). While few parameters have consistently large sensitivity indices for all output metrics, the majority of them have a significant influence only on few output metrics.

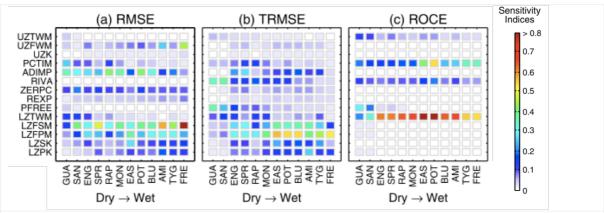


Figure 6. Example of using GSA to analyse the parameter influence of a hydrological model when applied in different sites (taken from van Werkhoven et al., 2008). Sensitivity of three different error metrics (RMSE, TRMSE, ROCE) to the 14 model parameters of a rainfall-runoff model applied to 12 catchments in the US. Catchments (on the horizontal axis) are sorted from drier to wetter climate. The plots show that sensitivity changes with the error metric but also from one catchment to another. Some patterns seem to emerge: for example, when moving from dry to wet catchments, the RMSE sensitivity to parameter UZFWM (upper zone free storage) increases and the sensitivity to PCTIM (percent of impervious area) decreases. The explanation is that in wet catchments flow peaks predictions (which control RMSE) are more often generated by saturation of the upper zone free water storage, while in dry catchments peaks are mainly controlled by direct runoff from impervious areas. Another pattern easily interpretable is that of the parameter RIVA (riparian vegetation area), which has no influence on RMSE but an increasing influence on TRMSE in dry catchments. The explanation is that riparian vegetation mainly control evapotranspiration, which in turn has little impact on high flows (which control RMSE) and a greater impact on low flows (which control TRMSE) especially in dry watersheds. Further discussion and interpretation of other sensitivity indices can be found in van Werkhoven et al. (2008).

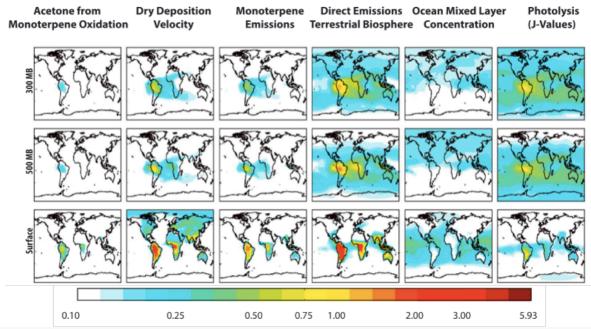


Figure 7. Example of using GSA to analyse the influence of parameters on spatially distributed output (taken from Brewer et al., 2017). Columns correspond to six input parameters of a global 3-D chemical transport model. Rows correspond to different outputs, i.e. acetone mixing ratios in three atmospheric layers. Range of variation of the sensitivity index exceed 1 because of the specific GSA method employed (Morris method, see e.g. Pianosi et al., 2016) however the interpretation is the same as in other Figures, i.e. the higher the index the more influential the input factor. The plots reveal that sensitivity changes massively across the spatial domain.

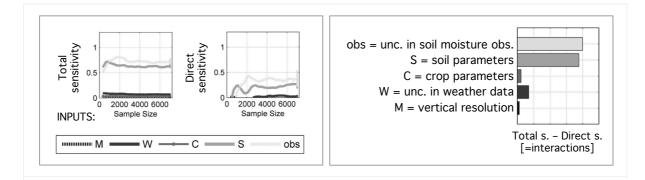


Figure 8. Example of using GSA for investigating the relative influence of uncertainty in parameters and in the observations of simulated variables of a soil-water-plan model (authors' re-elaboration of figures in Baroni and Tarantola (2014)). Left: 'total sensitivity' indices provide a measure of the overall influence of each factor on the error metric (root mean squared error between soil moisture predictions and observations) and 'direct sensitivity' indices measure the direct influence only, i.e. without considering interaction effects. Both 'direct' and 'total' sensitivity indices are evaluated using an increasing number of samples in order to assess their convergence. The plot shows that uncertainty in soil moisture observations (obs) and in soil properties (S) are dominant while other investigated input factors (crop parameters, meteorological forcing inputs, and chosen vertical resolution of the model) have a relatively negligible effect. Right: the difference between total and direct indices (evaluated at largest sample size) provides an indication of the level of interactions of each input factor with the others. Given the high difference values found for soil moisture observations and soil parameters, it can be inferred that the two must have a large amount of interactions with each other.



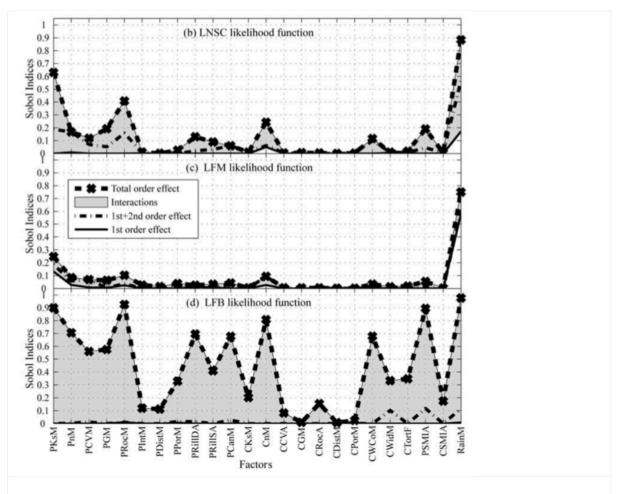


Figure 9. Example of using GSA for investigating the relative influence of uncertainty in parameters, initial conditions and input forcing data of a flow forecasting model (taken from Yatheendradas et al. (2008)). Each panel reports the sensitivity indices for a different error metric (LNSC, LFM, LFB). The input factors shown on the horizontal axis are the model parameters (acronyms starting by P), the model initial conditions (acronyms starting by C) and the rain depth bias factor (RainM) that is used to estimate rainfall rate from radar reflectivity observations. The example shows that the latter parameter has a very large influence on all error metrics and almost completely dominate the second one.

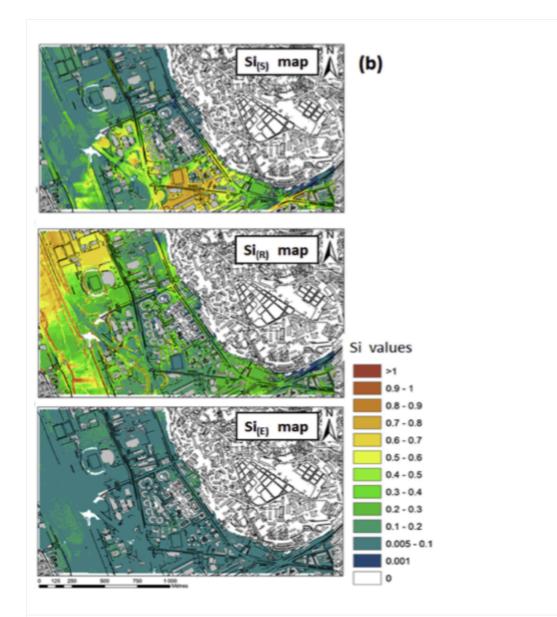


Figure 10. Example of using GSA for investigating the relative influence of measurement errors and discrete modelling choices for a flood inundation model (taken from Abily et al. (2016)). The panels show the spatial distribution of the sensitivity of water depth predictions to three uncertain input factors: chosen level of details in representing above ground features (top), resolution grid (middle), and measurement errors in high resolution topographic data (bottom). The figure highlights that the influence of different factors vary spatially but also that the modeller choices (first two panels) are overall much more important than measurement errors in this particular case.

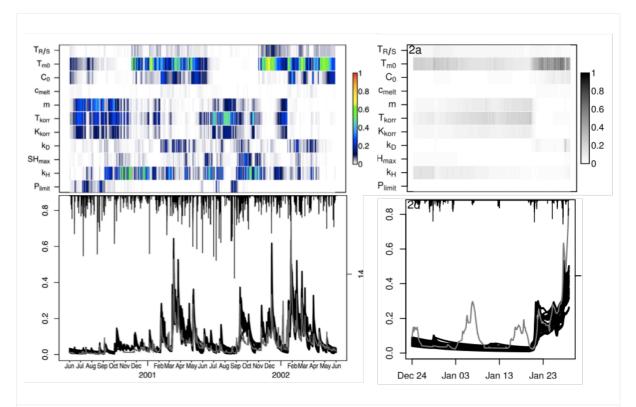


Figure 11. Example of using GSA for model validation (taken from Reusser and Zehe, 2011). The top panels show the temporal evolution of the sensitivity of flow predictions for the 11 parameters of a hydrological model (on the left the entire simulation period, on the right the zoom on selected days). To support interpretation, the bottom panel shows the time series of river flows (grey: observations; black: uncertain model predictions) and of rainfall forcing (from top) over the same periods. The left panels show an overall alignment between dominant parameters revealed by GSA and processes that are expected to dominate flow formation. For example, the top 3 parameters, which control snow accumulation and melt dynamics, are only influential in periods of the year when those processes are expected to occur. Another example is the fourth parameter from the bottom (kd), which is the recession constant for surface runoff and is only influential after large flood events. The right panels focus on a period (between January 3 and January 23) where the model fails to reproduce two observed flow peaks events. The missing sensitivity to the temperature melt index (third parameter from the top, C₀) indicates that no snowmelt can occur in the model during this period, and therefore the mismatch between predictions and observations must be attributed to a model deficiency (for example, the exclusion of radiation-induced melt processes) or a misinterpretation of flow observations (for example, rises in river flow caused by backwater effects due to ice jams).

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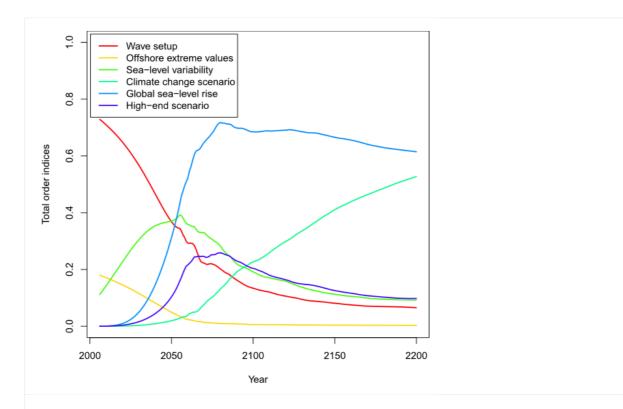


Figure 12. Example of using GSA to support long-term assessment of coastal defences (taken from Le Cozannet et al., 2015). The Figure shows the temporal sensitivity of predicted coastal defence vulnerability (specifically the output metric is the yearly probability of exceeding the threshold height of coastal defences). The figure shows that dominant drivers change significantly over time, for example global climate change scenario only matters beyond 2070 while offshore extreme values have no influence after then. Interestingly, for the time period up to 2050 the dominant factor is the 'wave set-up' parameter, which accounts for sea level rise induced by wave breaking. This is a local process determined by the near-shore coastal bathymetry and often neglected in coastal hazard assessments studies. GSA reveals that failing to incorporate the uncertainty in this process may invalidate conclusions and lead to an overestimation of the effects of other drivers at least on short and mid-term planning period.

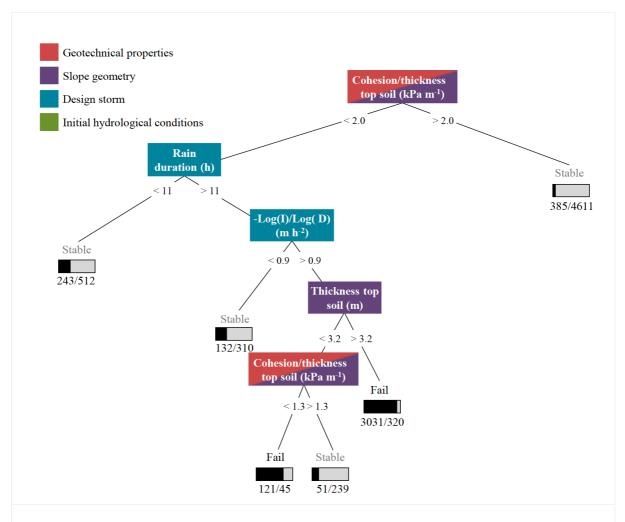


Figure 13. Example of using GSA to implement a 'bottom-up' approach to decision-making in the presence of unbounded uncertainties (taken from Almeida et al. (2017)). A Classification And Regression Tree (CART) is used to map the input factors of a hillslope scale landslide model onto model outcomes that are above (slope fails) or below (slope stable) a critical threshold of the so-called "factor of safety". Each coloured node corresponds to one of the analysed uncertain input factors, which include model parameters (geotechnical and geometrical slope properties), initial conditions and design storm characteristics (rain intensity and duration). The bars at the end of each branch show the proportion of simulations that resulted in slope failure (black) or stability (grey) for that leaf. The CART also displays the critical threshold values that cause a transition from one class to another (< >).