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Framework for setting up a Hydro-JULES perturbed parameter ensemble (PPE)

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1 Introduction

Land surface and hydrological processes and feedbacks that act at sub-grid scales need to be parameterised within models. These parameterisation schemes are an important source of uncertainty in model simulations. One of the aims of Hydro-JULES (HJ) is to quantify uncertainties in river flows induced by land surface and hydrological model parameterisations.

All models contain adjustable parameters, and each individual parameter can have a significant impact, depending on the model's sensitivity to that parameter, on the model outputs. Some parameters can be directly measured (such as height of vegetation) while others are estimated (or calibrated) using manual or automated trial and error techniques comparing the model output to wider-scale observations (such as river flow). Both types of parameters (measured and estimated) can be subject to considerable uncertainty and the model may be more or less sensitive to them in different climate conditions. The most thorough way to investigate model parameter uncertainty is by using a perturbed parameter ensemble (PPE).

The scientific motivation for using a PPE in Hydro-JULES is (a) to quantify uncertainty in predictions of soil moisture, river flow, etc; (b) to partition uncertainty between its sources; and (c) to attribute uncertainty to particular parameters in order to identify productive areas for future research. This guidance note outlines considerations for setting up a PPE to facilitate assessments of the uncertainties arising from the parameter values in HJ configurations.

2 PPE definition and previous studies

A PPE is one where physical parameters from different parts of a model are systematically perturbed within expert-specified ranges to form different 'realisations' of the model (also referred to as ensemble members). To constrain the parameter range, model developers typically conduct a sensitivity analysis to see how the outputs of the model vary with alterations to each parameter. A PPE differs from a sensitivity analysis because ensemble members are considered to produce valid forecasts/projections whereas in a sensitivity analysis parameter bounds can be pushed without necessarily considering validity. PPE parameters can either be fixed (Murphy et al. 2004, Hacker et al. 2011) or vary randomly in time (Bowler et al. 2008). The key strength of the perturbed parameter approach is the ability to produce a large set of ensemble members relatively easily (Collins et al. 2011).

PPEs differ from the other two main types of ensemble; initial condition (IC) and multi-model ensembles (MME). For an IC ensemble each ensemble member has the same set of parameter values, but a different starting state, and MMEs sample uncertainties using multiple models with different parametrisations schemes or model structures. PPEs should be seen as complimentary to multi-model and IC ensembles.

PPEs have been widely used for global-scale climate modelling studies, notably within the climateprediction.net (Murphy et al. 2004; Stainforth et al. 2005) and Met Office Quantifying Uncertainty in Model Predictions (QUMP) projects (Murphy et al.

2004), and for mesoscale (Hacker et al. 2011) and convection-permitting (Gebhardt et al. 2011; Vié et al. 2012; Baker et al 2014) ensemble systems. Many studies have focussed on perturbing atmospheric parameters in order to gain an understanding of the drivers of uncertainty in climate sensitivity and regional climate change, however to provide robust information on risks a more comprehensive sampling of uncertainties is required. Some studies have used PPEs for investigating uncertainties due to land surface parameters (CLMCUBE; Fischer et al. 2011; Cloke et al. 2011; Booth et al. 2012; Boulton et al. 2017) and in hydrological models (Wilby 2005; Smith et al. 2019). PPEs have also been used to quantify uncertainties in climate extremes, such as heat waves (Clark et al. 2006; Barnett et al. 2006), wet days (Barnett et al. 2006) and droughts (Burke and Brown 2008). The new UK Climate Projections (UKCP18) provide a 15-member global PPE (~60km) and a 12-member (~12km and ~2.2km) regional PPE (RCM-PPE) over the UK (Murphy et al. 2019).

PPE results depend on the design of the perturbation strategy (fixed, time-varying, random selection, all combinations), as well as on the base model used in the PPE. PPEs can be used for a range of applications including refining parameter sets (Williamson et al. 2013, Li et al. 2019) and studying transient model drifts (Mulholland et al. 2017).

Doug McNeall (Met Office and Univ Exeter) has estimated the range of uncertainty in the carbon cycle using a perturbed parameter ensemble (McNeall, 2019a, 500 ensemble members, 32 carbon cycle parameters). He looked at how the input values corresponded to important output values (e.g. NPP, runoff). By using weak constraints he has been able to reduce the parameter space and identify which parameter ranges give a reasonable carbon cycle and could be used to build an emulator (statistical model, McNeall, 2019b). Initially he tested doubling or halving parameter values to create a large hypercube this led to some model runs failing (it’s easy to kill the carbon cycle) and others not meeting his constraints (e.g. producing runoff > 0).

Cooper et al. 2021 found optimal values of constants in the pedotransfer functions which relate soil texture to soil parameters in the Joint UK Land Environment Simulator (JULES) land surface model. This has been achieved by using COSMOS-UK data within a data assimilation system (LaVEnDar, Pinnington et al. 2020).

3 Parameter values

When designing a PPE there are practical considerations concerning the number of parameters that can reasonably be perturbed, how to change the parameters for each model run, and the number of model runs that could be carried out. During the testing of a potential HJ module a sensitivity analysis should be performed to identify which parameters the module output is most sensitive to. During this test the upper and lower bounds of the parameters can also be explored. Sensitivity analyses may follow a “one at a time” (OAT) approach (e.g. Daniel 1973), or a more complex technique such as Sobol’ analysis (Sobol’, 1993), or Fourier Amplitude Sensitivity Testing (FAST, Cukier et al 1978). There are frameworks for model calibration and post-calibration uncertainty analysis (e.g. PEST – Model-Independent Parameter

Estimation, Doherty 2015) that could be used to explore the parameter space. It is generally considered that there can be no single correct or optimal model and different sets of model parameters may lead to equally good model performance (known in the literature as the “equifinality” concept, Beven 1993). Methods such as GLUE (Generalised Likelihood Uncertainty Estimation, Beven and Binley 1992) and MCMC (Markov Chain Monte Carlo) can however be used to generate plausible sets of parameter values.

For each tuneable parameter identified in the sensitivity analysis, a default value, a lower and upper band and a distribution function should be supplied (Table 1). Along with comments (including any references) on how the values have been agreed e.g. sensitivity testing, observations etc. Where sets of reasonable parameter values have been identified these can be used to generate the different PPE ensemble members.

Note, it is important that the module code is written in such a way that it is easy to change the parameter values, e.g. through a namelist or control file. Hard-coded parameter values must be avoided.

Table 1 *Parameter requirements*

Parameterisation scheme/module	Parameter name	Distribution function	Minimum value	Default value	Maximum value	Units	Comment

3.1 Techniques for generating the parameter sets

It is plausible to use all possible combinations of each parameter when considering a small number of parameters, however as the number of parameters to be perturbed increases it becomes necessary to sub-sample the parameter space to reduce computational cost. The most common ways to select parameter values within the PPE code are randomly (e.g. Monte Carlo simulations) or semi-systematically (e.g. Latin Hypercube Sampling).

One random method is the Monte Carlo technique which randomly selects parameter values from their probability distribution functions and randomly pairs them with other selected parameter values to form parameter sets (Wilby 2005). Although the Monte Carlo method is easy to implement, many thousands of model simulations are usually required to comprehensively sample the parameter space. One way to limit the number of simulations is to adopt a quasi-random parameter perturbation approach (e.g. Orth 2016). Another method, the random parameters scheme (Bowler et al. 2008), used in the Met Office Global and Regional Ensemble Prediction System (MOGREPS), evolves each parameter in time with an auto-regressive process to add stochasticity.

A popular systematic method is Latin Hypercube Sampling (LHS) which was designed to approximate the Monte Carlo method while using far fewer computational resources (McKay et al. 1979). Each probability distribution function is broken into intervals of equal probability from which one parameter value is selected and matched randomly with other model parameter values to form parameter sets. The number of required simulations is simply the number of equal-probability intervals selected; therefore, any number of model parameters can be perturbed without increasing the number of simulations. Examples of PPE studies that have used LHS to generate parameter sets are MacDougall et al. (2016) who estimated the release of carbon from permafrost soils, Boulton et al. (2017) who explored the effect of uncertainties in climate and land surface processes on the future of the Amazon rainforest, and Smith et al. (2019) who estimated hydrological model uncertainty in UK catchments.

4 Other considerations

Advantages of PPEs

- Designed to sample uncertainties within a single model framework in a systematic fashion.
- Can run many different simulations, only limited by the computational cost.
- PPEs only use one base model so eliminate the need to develop and maintain completely different models therefore resources can be devoted to finding optimal sets of parameters for the default parameterisation schemes.

Disadvantages of PPEs

- Results will depend on the design of the perturbation strategy, as well as on the base model itself.
- PPEs do not typically explore uncertainties in model structure such as the choice of resolution or alternative approaches for parameterising sub-grid scale processes.
- Results from a PPE are inherently probabilistic and not deterministic, which is not always appropriate for end-users.
- Once accepted parameterisations are determined from the PPE, the number of ensemble members may be prohibitive in the computational demand for future experiments (e.g. large climate change experiments).

Questions/discussion points for module developers

- What are we targeting?
    - *Feedback - river flow and soil moisture*
- Do we want to consider non-dimensionalising the model?
- How many ensemble members can/should be run?
- Ensemble size vs computational cost.
    - How many parameters should be perturbed?
    - In which parameterisation schemes/modules? – prioritise?
    - Do we want to randomly select the parameter values within the range or run all combinations?
    - Joint distribution of parameters – how to handle that?
- What sort of sensitivity testing should be carried out to determine the parameter ranges?
- Do we want parameters to be constant or varying in time?

    - *Feedback – keep them constant in time*
- A PPE would need to allow for different modules to be switched on (i.e. simple vs complex configurations) therefore each module that might be included in a PPE would need to have the parameters defined as in Section 3.
    - The ‘standard’ HJ configuration PPE would be simpler to define than one where the modules are selected based on the application.

Suggested way forward

- Each HJ parameterisation scheme/module to have a list of parameters and include a comment on how their values have been agreed (e.g. sensitivity testing, observations etc.). Include references where available (e.g. Table 1).
- Each HJ module (e.g. evaporation or river routing) to have a signature map to show how the subroutines and variables link together. This could then be extended to a HJ model which would consist of choosing multiple modules from the HJ framework.
- HJ developers to comment on the questions/discussion points above.

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