



*QUICS: Quantifying Uncertainty in  
Integrated Catchment Studies*

*2.1 Software tools for quantifying  
uncertainty across different scales*

Lead Partner: WU  
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## Report Details

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## Acronyms and Abbreviations

CRAN	Comprehensive R Archive Network
EAWAG	The Swiss Federal Institute of Aquatic Science and Technology (German acronym for Eidgenössische Anstalt für Wasserversorgung, Abwasserreinigung und Gewässerschutz)
FE	Finite elements
GSA	Global Sensitivity Analysis
ICM	Integrated Catchment Modelling
JLU	Justus Liebig University
LHS	Latin hypercube sampling
MC	Monte Carlo
MCMC	Markov Chain Monte Carlo
pdf	Probability density function
QUICS	Quantifying Uncertainty in Integrated Catchment Studies
spup	Spatial uncertainty propagation
SRS	Simple random sampling
SWMM	Storm Water Management Model
UQ	Uncertainty quantification
VBA	Visual Basic Application
WDF	Water Framework Directive
WQ	Water Quality
WU	Wageningen University

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## Executive Summary

The aim of this report was to:

- (1) identify and give an overview of the development of tools that can be used to propagate errors in integrated catchment studies across different spatial and temporal scales;
- (2) provide an overview of the software platforms used within QUICS;
- (3) present the motivation for and progress on development of the (spatial) uncertainty propagation analysis R package.

A number of tools for uncertainty quantification have been presented. There exists a wide selection of different uncertainty quantification software platforms, each of them having unique strengths and weaknesses and being suitable for different kind of problems. However, only few of them contain comprehensive toolsets for carrying out the entire uncertainty propagation assessment process, have universal applicability, are extendible and easy to use by non-experts.

Due to high popularity of programming languages R, Python and MATLAB, the uncertainty studies within QUICS relied exclusively on these programming platforms. The main motivation for using these platforms were: free software, open-source, sharable code (R, Python), widely used (R, Python, MATLAB), strong statistical functionality (R) and control over own code (R, Python, MATLAB).

Environmental variables vary in space and time. The space variation is often displayed by a mean of maps created using various interpolation techniques and thus naturally encumbered with interpolation errors. The patterns of uncertainty in space are important because the impacts of correlated error may differ substantially from those associated with random error. To bring the spatial (and non-spatial) uncertainty propagation analysis methods to a wider audience QUICS partner Wageningen University is developing an R package (spup) that will provide functions for analysing all main aspects of spatial uncertainty propagation, namely: (i) data uncertainty propagation, (ii) model parameter uncertainty propagation (iii) model structure uncertainty propagation (iv) contributions for propagated uncertainty, and (v) summary and visualization tools. The tool is intended for researchers and practitioners who understand the problems of uncertainty in data and models, and are looking for a simple, accessible implementation of the universal methodology for uncertainty assessment. At the same time, it is designed to enable more experienced users to easily understand, customise, and possibly further develop the code.

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# 1 Introduction

## 1.1 Background

According to the EU Water Framework Directive (WFD) each member country of the EU is required to ensure that water bodies achieve a good ecological status. In this context, it is important to be able to predict the impact of interventions on water quality (WQ). Man-made and natural processes control surface water quality. The WQ system is highly complex with a range of sources, transport and transformation processes. Cost estimates by EU governments indicate that billions of euros are being spent to implement the WFD. There is an increasing level of concern on the implementation cost (financial and environmental). Integrated water quality models designed to predict the quality of water across the linked urban and rural scales in a catchment are seen as tools to minimize these costs. Integrated Catchment Models (ICM) are based on linking multiple empirically calibrated sub-models of water quality processes. ICM are then used to evaluate potential measures and run scenarios. Current water quality sub-models contain significant uncertainties, with regard to model inputs, parameters as well as model structures. Methods have been developed to quantify uncertainty at the sub-model level, however little work has been carried out to investigate WQ uncertainty propagation between sub-models. Therefore, there is a need for development of a generalised catchment wide approach to uncertainty assessment that can be used in WFD implementation studies. This approach would address uncertainty propagation at the spatial and temporal scales found in catchments and develop tools to reduce uncertainty by optimising sampling and monitoring and the objective selection of model structure.

The European project QUICS (Quantifying Uncertainty in Integrated Catchment Studies) collates 12 PhD Candidates (Early Stage Researchers, ESR) and four postdocs (Experiences Researchers, ER) to perform quality research and collaborate with each other for developing and implementing uncertainty analysis tools for ICM.

## 1.2 Partners Involved in Deliverable

Wageningen University (WU)

Justus Liebig University (JLU)

## 1.3 Deliverable Objectives

This deliverable aims to provide an overview of available software for uncertainty quantification (UQ), applicability in QUICS and beyond, and lie in the motivation for development of a new UQ tool. Therefore the objectives of this report are:

1. Review of existing platforms for UQ.
2. Overview of current and planned usage of UQ tools within QUICS project.
3. Overview of the UQ tool (*spup* R package) developed at WU.

## 2 Obj. 1: Review of existing UQ platforms

There exist a plethora of different UQ platforms serving similar or different kind of tasks within UQ. The following selection of 18 platforms (Table 1) gives an overview of their functionality and applicability. We summarise each of the UQ platforms below.

Table 1 Existing software for uncertainty propagation analysis (based on Bastin et al. (2013)).

Platform	Full name	Author	Comments	Language	Availability	Application
@RISK		Palisade (2011)	Spreadsheet based.	Excel, VBA	commercial	Industry, environmental analysis (e.g. ecology)
COSSAN	COMputational Stochastic Structural Analysis	Schuëller and Pradlwarter (2006)	Implements finite elements methods for structural engineering.	MATLAB	commercial/free	Structural engineering
Crystal Ball		Oracle (2011)	Spreadsheet based.		commercial	Finance, marketing, engineering
DAKOTA	Design Analysis Kit for Optimisation and Terascale Application	Adams (2009)	Provides a flexible and extensible interface between simulation codes and the iterative built-in analysis methods.	C++	free	Fluid mechanics, structural dynamics, shock physics
DUE	Data Uncertainty Engine	Brown and Heuvelink (2007)	Quantification of positional and attribute uncertainty in environmental data by probability distributions that take spatial and temporal correlations into account. Can sample from these distributions for Monte Carlo uncertainty propagation analyses.	Java	free	Geography and environmental science
FRAMES/SUM3	Framework for Risk Analysis in Multimedia Environmental Systems	Gelston et al. (2008)	Monte Carlo analysis and Latin hypercube sampling. User supplies parametric distributions for input uncertainty (currently uniform, log-uniform, Normal, or log-Normal).		free	Environmental and human health impact
OpenTURNS	Open source initiative to Treat Uncertainties, Risks'N Statistics	Andrianov et al. (2007)	Powerful platform to perform uncertainty and sensitivity analysis.	Python	free	Engineering, structural mechanics
OSTRICH	Optimisation Software Toolkit for Research Involving Computational Heuristics	Matott (2005)	A versatile tool incorporating a diverse set of algorithms for calibration, optimisation and computation of statistics such as parameter correlation/sensitivity and observation influence.		free	Calibration of deterministic models
PEST	Parameter ESTimation	Doherty (2004)	Model-independent parameter estimation software for complex environmental and other computer models. Powerful calibration, regularization and optimisation toolkit. Implements a variety of parameter estimation methods, and null-space Monte Carlo approaches for linear and non-linear analysis of uncertainty propagation, parameter identifiability and error variance.	Fortran 90	free	Calibration of model parameters (e.g. waste water plume movement model)

Table 2 Continuation.

Platform	Full name	Author	Comments	Language	Availability	Application
PSUADE	Problem Solving environment for Uncertainty Analysis and Design Exploration	Tong (2005)	Provides an integrated design and analysis environment for performing UQ analysis of large complex system models. Runs only through command line languages (no GUI).	C++	free	Risk analysis, engineering
SAFE	Sensitivity Analysis For Everybody	Pianosi et al. (2015)	Application of Global Sensitivity Analysis.	MATLAB/Octave/R	free	Meteorology, hydrology, other environmental science
SimLAB		<a href="https://ec.europa.eu/jrc/en/samo/simlab#c2907">https://ec.europa.eu/jrc/en/samo/simlab#c2907</a>	Focuses on uncertainty analysis and sensitivity analysis. Provides a reference implementation of many global sensitivity analysis techniques.		free	Climate change, hydrology, nuclear science, engineering
TIME	The Invisible Modelling Environment	Rahman et al. (2005)	User supplies parametric distributions as above. Some visualization of uncertainty (e.g., confidence limits on outputs).	Fortran/C#	free	Environmental science, engineering
UCODE		Poeter et al. (2005)	Performs inverse modelling, posed as a parameter estimation problem, using non-linear regression approach. Like OSTRICH and PEST, generates confidence intervals and other statistics.	Fortran	free	Environmental science (e.g. ground water studies)
UNCSAM		Janssen et al. (1994)	Can do model emulation; does not cope with spatially and/or temporally correlated variables.	Fortran 77	free	Biogeochemistry, environmental pollution
UNCSIM		Reichert (2006)	Analyses the sensitivity of model results to model parameters.	C++	free	Calibration of deterministic models
UQLab	Uncertainty Quantification in MATLAB	Marelli and Sudret (2014)	Designed to be extended to the engineering research community. Mainly using non-intrusive stochastic methods as Polynomial Chaos Expansion (PCE).	MATLAB	free	Environmental and engineering science
R package 'propagate'		Spieß A.N. (2014)	Propagation of uncertainty using higher-order Taylor expansion and Monte Carlo simulation.	R	free	ecology

## 2.1 @RISK

@RISK ('at risk') is a spreadsheet based software for analysing risk and uncertainty in a wide variety of industries (Palisade, 2016). It is a commercial platform developed by Palisade Corporation as an add-in to Microsoft Excel (Figure 1). @RISK employs Monte Carlo (MC) methodology. The user defines uncertain cell values in Excel as probability distributions using functions (@RISK adds a set of new functions to the Excel function set, each allowing to specify a different distribution type for cell values). A function is provided to identify correlations between variables including correlation in time series. Only numerical variables are supported. Distribution functions are invoked during a simulation. @RISK has a capability for specifying and executing simulations of Excel models. Both simple random sampling (SRS) and Latin hypercube sampling (LHS) techniques are supported, and distributions of possible results may be generated for any



cell or range of cells in the spreadsheet model. Graphics are used to present the output distributions from the @RISK simulations including histograms, cumulative curves and summary graphs.

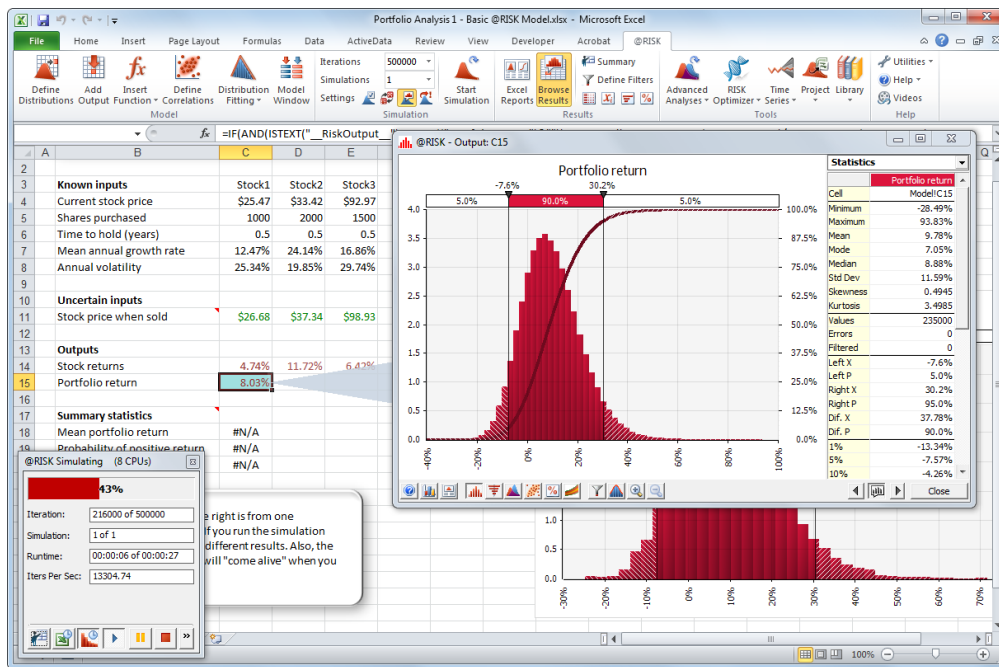


Figure 1 @RISK software interface (Palisade, 2016).

@RISK aims at a wide spectrum of industry as customers, however the number of users are not reported. Palisade (2016) proposes that, among others, the tool may be used for environmental analysis (e.g. case studies on endangered species preservation or pollution clean-up and projections). It has been used in one of DEFRA (Department for Environment, Food & Rural Affairs, UK) projects on pesticide fate modelling (Dubus et al., 2002). Both a free trial and a commercial version are available via [www.palisade.com](http://www.palisade.com).

## 2.2 COSSAN™

COSSAN™ (Computational Stochastic Structural ANalysis) is a software developed at the Institute of Engineering Mechanics of the Leopold Franzens University, Innsbruck, Austria (Schuëller and Pradlwarter, 2006). COSSAN is based on interaction with third party 'Finite Elements' (FE) tools. The FE method is a numerical technique for finding approximate solutions to boundary value problems for partial differential equations used for example in structural engineering. Two set of components, i.e., the 'Stand Alone Tool Box' and the so called 'Third Party Communication Tools', are available for providing stochastic structural analysis solutions, each serving particular needs and requirements. The 'Stand Alone Tool Box' is designed as an open modular general purpose software. In this implementation, all computational tasks are controlled and solved within the software. The 'Stand Alone Tool Box' covers a wide field of applications ranging from optimisation, fracture and damage analysis, random vibration, system identification, deterministic and stochastic FE-analysis, MC simulation to reliability assessment. Its usage requires significant efforts to get acquainted with the commands and possibilities of the 'Stand

Alone Tool Box'. Bridging the gap between deterministic and stochastic concepts is facilitated by applying MC simulation. To facilitate the coupling between the two concepts, the 'Third Party Communication Tools' have been developed. With these, stochastic analysis solutions based on MC simulation can be accessed while using available deterministic 'Third Party codes'.

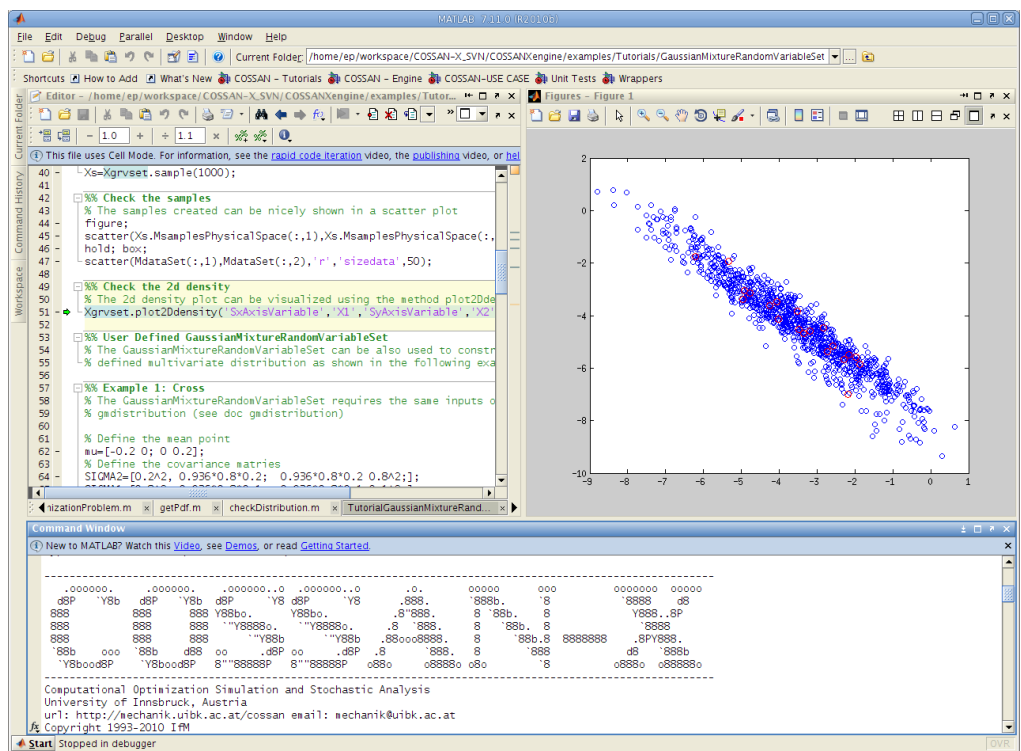


Figure 2 OpenCOSSAN™ software interface (<http://www.cossan.co.uk/software/open-cossan-engine.php>, accessed 4<sup>th</sup> May 2016).

The examples of applications in structural engineering include a satellite structure under harmonic excitation and a multi-storey building subjected to stochastic ground acceleration (Schuëller and Pradlwarter, 2006). The recent new implementation of COSSAN, namely COSSAN-X™, is coded in MATLAB (Valdebenito et al., 2010, Figure 2). The developers provide also a free of charge OpenCOSSAN version of the software (available at [www.cossan.co.uk](http://www.cossan.co.uk)).

### 2.3 Crystal Ball

The Crystall Ball software by Oracle (Oracle, 2011) is another commercial spreadsheet-based application (Figure 3) for predictive modelling, forecasting, simulation, and optimisation. The uncertainty quantification is based on MC simulations. The software is aimed to be used by strategic planners, financial analysts, engineers, scientists, entrepreneurs, marketing managers, venture capitalists, consultants, and anyone else who uses spreadsheets to forecast uncertain results.

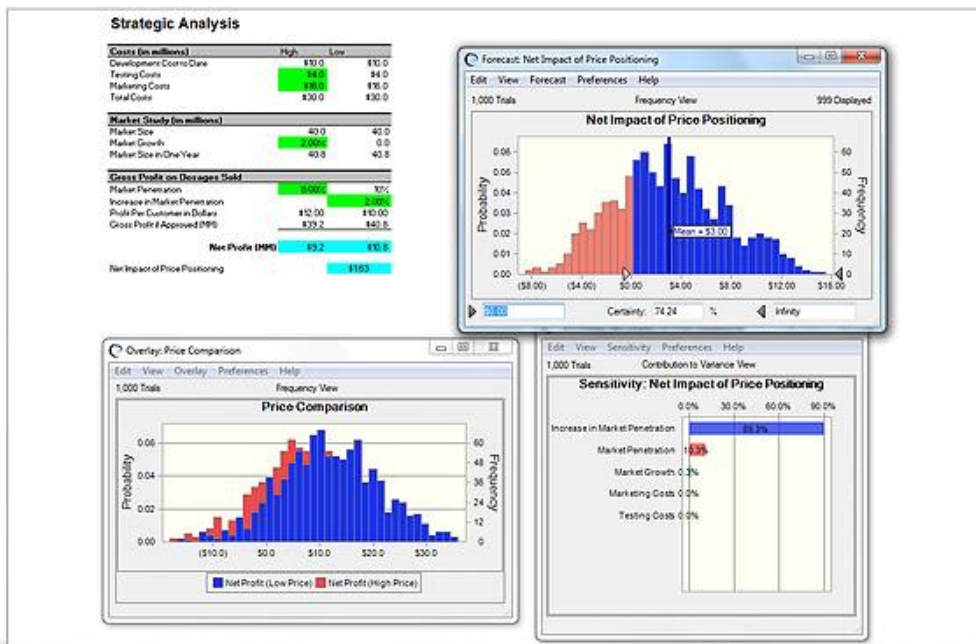


Figure 3 Crystal Ball software interface (<http://www.oracle.com/us/products/applications/crystalball/overview/index.htm>, accessed 4<sup>th</sup> May 2016).

## 2.4 DAKOTA

The Dakota (Design Analysis Kit for Optimisation and Terascale Applications) toolkit provides a flexible and extensible interface between simulation codes and iterative analysis methods (Adams et al., 2009). It has been developed in C++ by Sandia National Laboratories. Dakota contains algorithms for optimisation with gradient and non-gradient-based methods; uncertainty quantification with sampling, reliability, and stochastic expansion methods; parameter estimation with nonlinear least squares methods; and sensitivity/variance analysis with design of experiments and parameter study methods. These capabilities may be used on their own or as components within advanced strategies such as surrogate-based optimisation, mixed integer nonlinear programming, or optimisation under uncertainty. It is a dedicated environment for design and performance analysis of computational models on high performance computers. Uncertainty quantification in DAKOTA is related to sensitivity analysis for understanding of how variations in parameters affect the response functions of the engineering design problem. The methodologies include sampling-based approaches, i.e. random sampling and LHS, local and global reliability methods, and stochastic expansion (polynomial chaos expansions and stochastic collocation). Dakota operates on most systems running Unix or Linux operating systems as well as on Windows, natively in a Command Prompt window, and (optionally) with the help of a Cygwin emulation layer. The example of an input file for uncertainty quantification analysis, to be invoked from a command line, is shown in Figure 4.

```

# Dakota Input File: textbook_uq_sampling.in
environment
  tabular_graphics_data
  tabular_graphics_file = 'textbook_uq_sampling.dat'

method
  sampling
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
  fork async evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

```

Figure 4 Dakota input file for UQ example using LHS (Adams et al., 2009).

The software aims at engineering design field and scientific discovery activities for simulating complex physical systems in disciplines such as fluid mechanics, structural dynamics, heat transfer, nonlinear structural mechanics or shock physics. An example application on uncertainty quantification and data assimilation in a design of a nuclear reactor has been reported in (Hite et al., 2013). DAKOTA is free software available via <https://software.sandia.gov/trac/dakota/>.

## 2.5 DUE

The DUE (Data Uncertainty Engine) (Brown and Heuvelink, 2007) is a software tool for assessing uncertainties in environmental data, storing them within a database, and for generating realisations of data to include in MC uncertainty propagation studies. The functionality supported by DUE includes:

- a conceptual framework for guiding an uncertainty assessment, which is implemented through a graphical user interface (Figure 5);
- specification of a probability model for continuous numerical attributes, discrete numerical attributes and categorical attributes. The attributes may be constant or may vary in space and time;
- parametric probability density functions (pdfs) for continuous (e.g. normal, lognormal, Weibull) and discrete numerical data (e.g. Poisson, binomial, uniform), with the option to define a non-parametric pdf for discrete numerical and categorical data;
- the specification of correlations within a single object or attribute and cross-correlations between objects or attributes (only if the pdfs follow a joint normal distribution);
- aggregation of (uncertain) attribute values to larger spatial scales, including aggregation from points to blocks;
- efficient stochastic simulation from pdfs;

- import from and export to file (with a limited range of formats), as well as a 'DUE-enabled' database;
- use of the Java programming language, which is platform independent and may be executed on all operating systems that support a Java Virtual Machine.

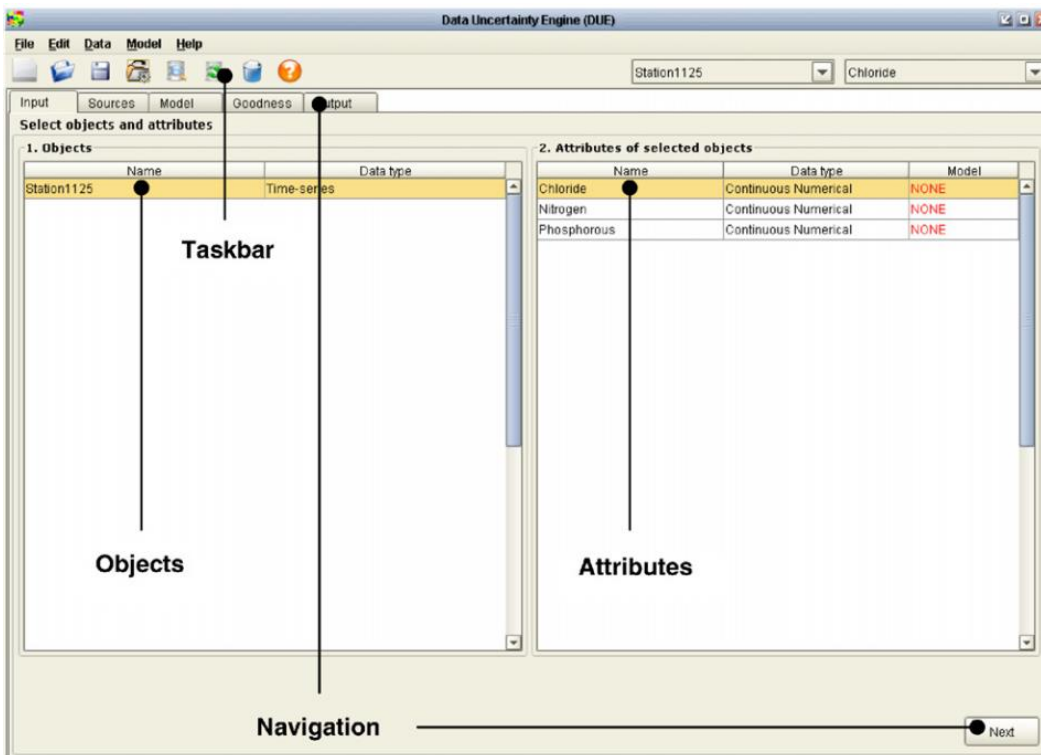


Figure 5 The opening window of DUE with a time-series object loaded (Brown and Heuvelink, 2007).

The software is intended for researchers and practitioners who understand the problems of uncertainty in spatial data and models but do not have the time or background in uncertainty methods to design their own study with more generic tools, such as R or MATLAB. The examples of application include uncertainty analysis of the GeoPEARL pesticide leaching model, uncertainty analysis of a regionalised water quality model or handling positional uncertainty in a spatial planning project (Heuvelink, 2007). The software is freely available through <http://www.harmonirib.com/download/DUE.htm>.

## 2.6 FRAMES/SUM3

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) software is designed by Pacific Northwest National Laboratory, US, for deterministic environmental and human health impact models (Gelston et al., 2008). The Sensitivity/Uncertainty Multimedia Modelling Module (SUM3) software product was designed to allow a statistical analysis using the existing deterministic models available in FRAMES. SUM3 is based on MC methodology and implements SRS and LHS for randomly sampling input variables. The sampling output values in an external file are available to the user for evaluation, e.g. calculating deterministic values with



variable inputs and producing a statistical distribution of results. A typical application of the uncertainty analysis is to indicate relative conservatism of the deterministic result. The example interface of SUM3 is shown in Figure 6.

Although SUM3 was originally developed as a sensitivity/uncertainty tool for use with the Multimedia Environmental Pollutant Assessment System (MEPAS©) (Gelston et al., 2008), it is not restricted to MEPAS© models. SUM3 can also be used with other deterministic environmental, such as the Generation II (GENII) software system, which is a Hanford environmental dosimetry system (Napier et al., 1988). Within FRAMES, SUM3 allows users to conduct a sensitivity and/or uncertainty analysis to understand the influence and importance of variability/uncertainty input parameters on constituent flux, concentration, and human health impacts. The sensitivity analysis can identify the key parameters that dominate overall uncertainty. Examples of applications include: parallelised use in the 3MRA pollutant fate model (Babendreier and Castleton, 2005) and linking FRAMES with R to calculate & visualize impacts of input uncertainty (Castleton et al., 2006b). The software is available free of charge from <http://mepas.pnnl.gov/FRAMESV1/download.stm>.

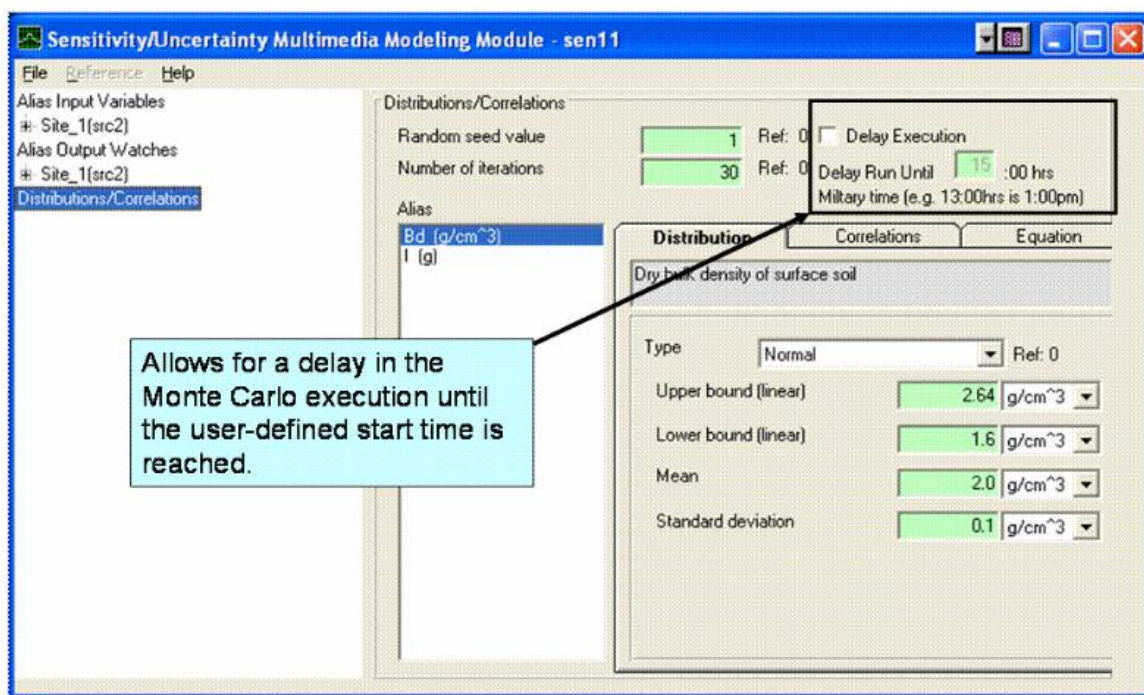


Figure 6 The Sensitivity/Uncertainty Multimedia Modelling Module interface (Castleton et al., 2006a).

## 2.7 OpenTURNS

OpenTURNS is an open-access software employing generic methodology for UQ, uncertainty propagation and sensitivity analysis (Baudin et al., in review). It has been developed collaboratively by several industrial companies and academic institutions including EDF R&D, Airbus Group, Phimeca Engineering and IMACS. The software is available as a scientific C++ library and a Python TUI, and works under Linux and Windows environments. A generic wrapper is also available to link OpenTURNS to any external code. OpenTURNS addresses the specific

industrial challenges attached to uncertainties, which are transparency, genericity, modularity and multi-accessibility and therefore mainly aims at engineers who want to introduce a probabilistic dimension to deterministic studies. The implemented UQ framework is based on quantification of the uncertainty sources, uncertainty propagation and ranking uncertainty sources/sensitivity analysis. Numerous methods are implemented for each of the steps including: empirical cumulative distribution function, Kernel smoothing, Maximum Likelihood and Bayesian Calibration for the quantification of the uncertainty sources; uniform random generator, distribution realizations, Taylor variance decomposition and MC simulations for uncertainty propagation; correlations coefficients, Sobol indices and Fourier decomposition for ranking uncertainty sources and sensitivity analysis. Detailed mathematical background and implementation of all methods can be found in the software Reference Guide (OpenTURNS, 2016b).

The examples of use are provided in the software documentation (OpenTURNS, 2016a). These include estimating uncertainty in deviation of a cantilever beam and elastic truss structure plus risk control study during flooding events (OpenTURNS, 2016b). The software download is available at <http://www.openturns.org/> and GitHub (<https://github.com/openturns/openturns>).

## 2.8 OSTRICH

OSTRICH (Optimisation Software Toolkit for Research Involving Computational Heuristics) (Matott, 2005) has been developed at the Department of Civil and Environmental Engineering, University of Waterloo and the Centre for Computational Research, University at Buffalo. OSTRICH has been created as a model-independent multi-algorithm optimisation and parameter estimation program that allows to automate the processes of model calibration and design optimisation. OSTRICH is model independent software and can be configured to operate with any modelling program that utilizes text-based input and output file formats. The optimisation software implements comprehensive collection of calibration algorithms, including uncertainty-based search algorithms (i.e. Generalized Likelihood Uncertainty Estimation (GLUE), Metropolis-Hastings Markov Chain Monte Carlo (MCMC)) as well as utilities for sensitivity and uncertainty analysis (i.e. regression statistics for local sensitivity analysis and user-specified model evaluations). OSTRICH is available for both Linux and Windows platforms and an MPI-parallel version of OSTRICH is available for Linux-based parallel clusters. Additionally, OSTRICH can be configured to execute parallel versions of the underlying model executable, if one is available. It is primarily designed to be run from a command line but an OSTRICH GUI module has been also developed using Visual Basic (Matott, 2005).

OSTRICH is primarily designed for researches and practitioners. It has been applied for calibration of multiple analytic element method groundwater flow models, with particular attention to effects of model precision and observation location (Rabideau et al., 2005). It was further used in applications for simultaneous calibration of equally plausible models by adaptive weighting and mapping of parameters between reference and surrogate models (Matott and Rabideau, 2008). The software can be downloaded free of charge from <http://www.eng.buffalo.edu/~lsmatott/Ostrich/OstrichMain.html>.

## 2.9 PEST

PEST is an open-source, public-domain software suite that allows model-independent parameter estimation and parameter/predictive-uncertainty analysis developed between Watermark Numerical Computing, S.S. Papadopoulos and Associates and Environmental Simulations Inc., Australia (Doherty, 2004). The platform is a model independent parameter estimation software for complex environmental and other computer models. It is a powerful calibration, regularization and optimisation toolkit. It implements a variety of parameter estimation methods, and null-space MC approaches for linear and non-linear analysis of uncertainty, parameter identifiability and error variance. It is accompanied by two supplementary open-source software suites for calibration of groundwater and surface-water models (Doherty, 2007, 2008). The PEST suite is comprised of two versions of PEST and six utility programs for building and checking PEST input files. A sensitivity analyser and a parameter pre-processor are also supplied with PEST. Similarly to Dakota (Section 2.4 these programs are command-line driven programs, i.e. they can be run from a command-line window by typing the name of the appropriate executable at the screen prompt calling appropriately formatted input files.

The PEST tools are heavily focused on parameter estimation, highly-parametrized inversion, and some uncertainty analysis: linear highly-parameterized parameter/predictive error variance assessment and uncertainty assessment; nonlinear, regularized, calibration-constrained parameter/predictive maximization/minimization; random parameter generation; MC analysis; predictive calibration analysis. The examples of PEST application include: integration of PEST into FRAMES software (Castleton and Meyer, 2009), testing of alternative hypotheses for the wastewater plume movement, by highly-parallelised calibration of candidate models and generation of a subset of 'superparameters' (Dausman et al., 2010) and description statistics (calculated using PEST) to summarise the extent to which each parameter of a model can be identified, and the extent to which the calibration process can improve on the estimate based on prior expert knowledge (Doherty and Hunt, 2009). PEST can be downloaded from <http://www.pesthomepage.org/Downloads.php>.

## 2.10 PSUADE

PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration) is a software system that can be used to study the relationships between inputs and outputs of general simulation models for the purpose of performing uncertainty and sensitivity analyses on simulation models (PSUADE, 2016). PSUADE is targeted for simulation models that are expensive to evaluate, such as large scale multi-physics models. The software has enriched sets of sampling and analysis tools. In addition, it has several robustness features for self-verifying the analysis results. PSUADE has been built as a C package, primarily for Unix or Linux-based systems. PSUADE is a mini-computational engine for supporting various uncertainty quantification activities such as forward and backward uncertainty analyses, sensitivity analysis, parameter exploration, model calibration, numerical optimisation and risk assessment. It supports mainly non-intrusive (simulation model as a black box) analysis although there is some capability for intrusiveness (e.g. derivative-based methods). PSUADE deals with dimension reduction (when the number of uncertain parameters in the system is large, it may be advantageous to filter out the less dominant



(sensitive) parameters before further processing), response surface analysis (representations of the relationships between the uncertain parameters and the outputs of interest) and uncertainty and sensitivity analysis.

Uncertainty analysis in PSUADE consists of generating a sample, propagating the sample through the models, and computing summary statistics. The software provides a rich set of sampling designs for such purpose. It supports a number of variance-based global sensitivity analyses: first order, second order, group order and total order. In addition, these analyses can be done on an arbitrary parameter space (after model calibration). Parameter estimation/inference uses either numerical optimisation (to obtain a single point) or Bayesian methods (to obtain posterior distributions) given a data set to form the objective (or likelihood) function. PSUADE provides a number of numerical optimisation methods. Also, PSUADE provides a MCMC algorithm for Bayesian inferences that use response surfaces.

PSUADE has some capabilities for risk analysis, namely to locate the failure threshold boundaries and has many visualization and data manipulation tools to facilitate UQ studies (Lin et al., 2012). The graphics are supported primarily through MATLAB scripts.

PSUADE has been applied in studies of sensitivity analysis of an engineering application (Hsieh, 2007). The software is free to download from [http://computation.llnl.gov/casc/uncertainty\\_quantification/](http://computation.llnl.gov/casc/uncertainty_quantification/).

## 2.11 SAFE

SAFE (Sensitivity Analysis For Everybody) is a MATLAB/Octave toolbox for the application of Global Sensitivity Analysis (GSA) (Pianosi et al., 2015) developed at University of Bristol, UK. It implements several established GSA methods and allows for easily integrating others. All methods implemented in SAFE support the assessment of the robustness and convergence of sensitivity indices. SAFE includes numerous visualisation tools for the effective investigation and communication of GSA results. The tool has a modular design (Figure 7) that allows plugging-in new code and using portions of the code only.

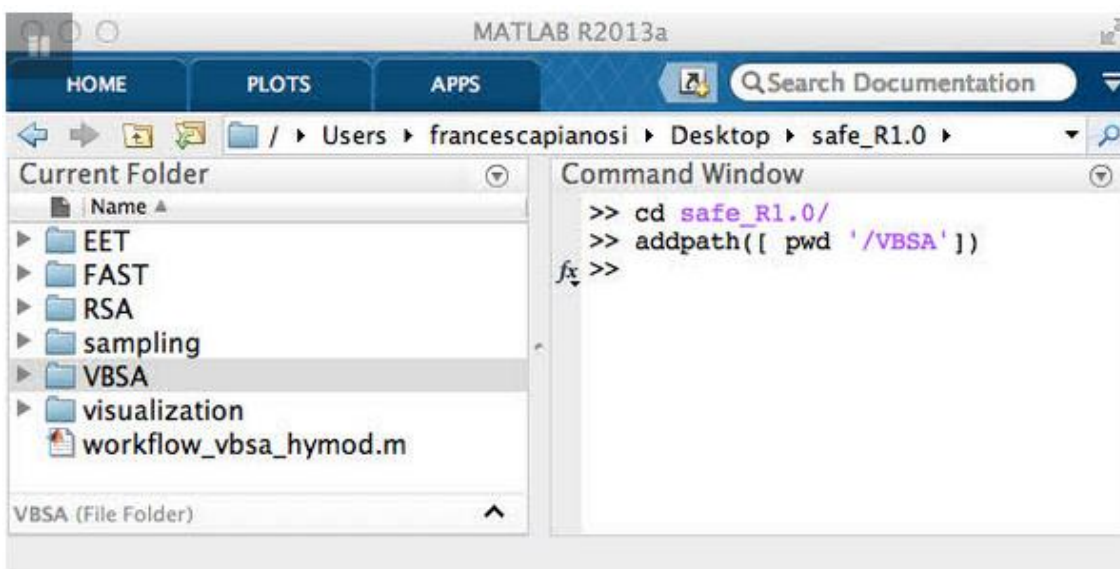


Figure 7 The modular structure of SAFE (University of Bristol, 2016).

The toolbox is designed to make GSA accessible to non-specialist users, and to provide a fully commented code for more experienced users to complement their own tools. The documentation includes a set of workflow scripts with practical guidelines on how to apply GSA and how to use the toolbox (Figure 8). An R-version of the Toolbox is also available. SAFE is open source and freely available for academic and non-commercial purpose and can be obtained by contacting the authors.

```

78
79 %% Step 3 (sample inputs space)
80 SampStrategy = 'lhs' ; % Latin Hypercube
81 N = 3000 ; % Number of samples
82 M = length(DistrPar) ; % Number of inputs
83 X = AAT_sampling(SampStrategy,M,DistrFun,DistrPar,N);
84
85 %% Step 4 (run the model)
86 Y = model_evaluation(myfun,X,rain,evap,flow) ;
87
88 %% Step 5a (Regional Sensitivity Analysis with threshold)
89
90 % Visualize input/output samples (this may help finding a reasonable value
91 % for the output threshold):
92 scatter_plots(X,Y(:,1),[],'rmse',x_labels) ;
93 scatter_plots(X,Y(:,2),[],'bias',x_labels) ;
94
95 % Set output threshold:
96 rmse_thres = 3 ; % threshold for the first obj. fun.
97 bias_thres = 0.5 ; % behavioural threshold for the second obj. fun.
98
99 % RSA (find behavioural parameterizations):
100 threshold = [ rmse_thres bias_thres ] ;
101 [mvd,idxb] = RSA_indices_thres(X,Y,threshold) ;
102

```

Figure 8 Documentation is embedded in the code throughout comments and a set of workflow scripts to get started (University of Bristol, 2016).

## 2.12 SimLAB

SimLab offers a free programming and development environment developed by the Econometrics and Applied Statistics Unit of the European Commission and aims to facilitate the integration of sensitivity analysis features into user's modelling software (SimLab, 2008). It is a software package type: C++ shared library (i.e., a WIN32 DLL or a Shared Object for UNIX/POSIX) or binary distribution with Install Shield on Microsoft Windows 32-bit (Figure 9). SimLab is designed to be used as a black-box and it needs to be "hosted" within the user's application. The user invokes SimLab via calls to DLLs (for UA/SA methods) within either one of Fortran, C/C++, or MATLAB environments. Supported techniques include: uncertainty analysis (min, max, mean, variance, histograms; skewness; kurtosis, Kolmogorov, Tchebycheff's and T test), sensitivity analysis (via distributions: continuous and discrete densities, as well as constant and relation factors; sample generation: random, quasi-random LpTau, LHS, FAST, Morris and Sobol indices). It allows for output evaluation via various metrics including: scatterplots; Pearson product moment correlation coefficient, partial correlation coefficients, standardized regression coefficients; Spearman rank correlation coefficient, partial rank correlation coefficients, standardized rank regression coefficients; importance measures, Morris and Sobol indices.

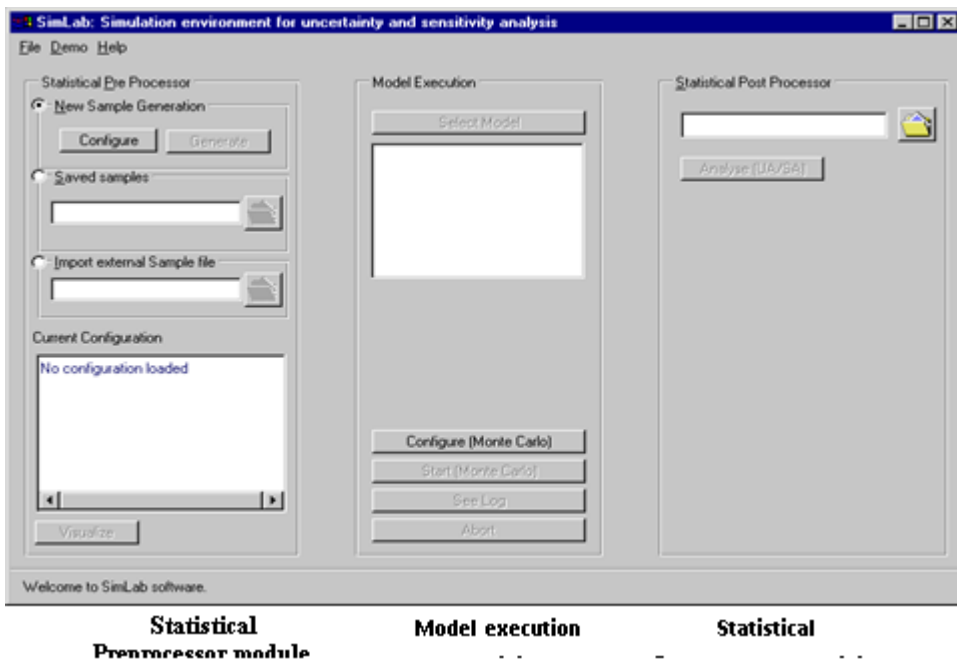


Figure 9 SimLAB main panel (SimLab, 2008).

The application is mainly focused on developing new methods in sensitivity analysis, for example: application of non-parametric methods for global sensitivity analysis of model output with dependent inputs (Mara et al., 2015), transformations and invariance in the sensitivity analysis of computer experiments (Borgonovo et al., 2014) or application of the control variate technique to estimation of total sensitivity indices (Kucherenko et al., 2015). The full list of references to SimLAB applications can be found at the software website <https://ec.europa.eu/jrc/en/page-related-publications-list/all/572/33434>. SimLab can be downloaded from <https://ec.europa.eu/jrc/en/samo/simlab>.

## 2.13 TIME

The Invisible Modelling Environment (TIME) is a .NET based model development framework, supporting model developers in the creation and testing of algorithms and in the development of standalone modelling applications (Rahman et al., 2005). TIME underpins the modelling products in the Catchment Modelling Toolkit (eWater, 2016); a community developed collection of water quantity, water quality and related models. TIME is founded on a compact architecture with a series of subsystem frameworks, handling issues such as data visualisation and non-linear optimisation. The software supports the areas of spatial and temporal data analysis where a series of GIS-like tools and novel algorithms have been implemented. Additionally a series of generic, non-linear optimisation tools have been incorporated and used in several toolkit products. A visual tool for the integration of models has also been included. The underlying framework has been extended to include the representation and visualisation of data uncertainty.

Data uncertainty is defined as the representation of the uncertainty for each of its items (time series or rasters), i.e. by assigning a pdf for each data item. Data uncertainty may hence range from being simply described as a Gaussian pdf centred on each item value and with a standard deviation that is a fraction of this item value, or a complex pdf derived running a MC simulation and summarising the characteristics of the realisations for each data item. Visualisation of data uncertainty is supported for time series data principally. Spatial uncertainty visualization is not supported.

The software serves as the development platform for approximately 50 model developers from a range of technical backgrounds, from professional software developers to PhD hydrologists (Searle and Penton, 2012), however the literature on the application is limited. An example of application is presented in Rahman et al. (2005). The Stochastic Climate Library draws on the framework's inbuilt capabilities for visualisation, data handling and temporal analysis to create a polished modelling product producing stochastic climate replicates. This library includes a collection of models, which already existed in various forms, and a number of approaches were used to bring them into TIME, including porting to newer dialects of the original language (Fortran), wrapping as DLLs, and porting to C#, a language with additional capabilities. The software is free to download via the eWater website (<http://www.toolkit.net.au>).

## 2.14 UCODE

UCODE was developed to perform inverse modelling, but also includes sensitivity analysis; data needs assessment; calibration; prediction; and uncertainty analysis (Poeter et al., 2014). It has been developed in Fortran 90/95 by the U.S. Geological Survey. Any application model or set of models can be used; the only requirement is that they have numerical (ASCII or text only) input and output files and that the numbers in these files have sufficient significant digits. Application models can include pre-processors and post-processors as well as models related to the processes of interest (physical, chemical and so on) (Poeter and Hill, 1999). The limitation in the software is that it uses only local, and not global, methods for sensitivity analysis. Otherwise the functionality includes: manipulating application model input files and read values from application model output files; comparing user-provided observations with equivalent simulated values derived from the values read from the application model output files using a weighted least-squares objective function; using a modified Gauss-Newton method to adjust the value of user selected input parameters in an iterative procedure to minimize the value of the weighted least-squares objective function; reporting the estimated parameter values; calculating and printing statistics for:

- diagnosing inadequate data or identify parameters that probably cannot be estimated;
- evaluating estimated parameter values;
- evaluating how accurately the model represents the field processes;
- quantifying the uncertainty of model predictions.

Uncertainty evaluation is done using MCMC techniques. Inclusion of MCMC uncertainty measures results in three methods of uncertainty evaluation in UCODE\_2014 that proceed from (i) linear uncertainty intervals that are very computationally frugal (commonly 10s to 100s of parallelizable model runs) and depend on the model not being too nonlinear and errors being approximately Gaussian, to (ii) nonlinear uncertainty intervals with moderate computational demands (commonly

1,000s of model runs) and depend on model smoothness and Gaussian errors, to (iii) MCMC uncertainty intervals that are computationally demanding (commonly 10,000s of model runs and more) and few restrictive assumptions (Poeter et al., 2014).

The example of application in groundwater model calibration is presented in Lu et al. (2012). The software can be obtained from <http://igwmc.mines.edu/freeware/ucode/>.

## 2.15 UNCSAM

UNCSAM (Janssen et al., 1994) is a tool for automating sensitivity and uncertainty analysis developed at the National Institute of Public Health and Environmental Protection (RIVM) in the Netherlands as an alternative to @RISK and Crystal Ball (Sections 0 and 2.3). UNCSAM can be used to analyse a broad spectrum of (simulation) models, largely independent of their form and implementation. Basic components comprise a collection of programs, developed for the various activities needed in sensitivity and uncertainty analysis (sampling and basic statistical analysis, confidence bounds for estimated quantities, determination of sensitivity and uncertainty contributions). Additional programs are available for UNCSAM-model interfacing, file manipulation (reading, selecting signals from data files), graphics etc. Sampling can be done from continuous probability distributions (i.e. (log)uniform, (log)normal, (log)triangular, exponential, logistic, Weibull, Beta). Sampling methods include SRS and LHS. User-specified parameter correlations are taken into account. Sensitivity and uncertainty contributions can be evaluated by a number of measures, based on linear regression and correlation analysis of the original and the rank-transformed data values.

UNCSAM generates a large number of files, containing data or information needed in the various stages of the analysis process. The storage load is constrained and loss of accuracy is avoided by storing intermediate numerical results in binary files. The final results (tables and plot instructions) are stored in ASCII-files. UNCSAM is developed in a model independent way, irrespective of how the user's model is implemented. This means that the user has the flexibility to use the package for many application studies, but needs to establish an interface between UNCSAM and his/her model. The function of this interface is to pass data files (of desired format) from the package to the model and vice versa. To enhance ease of use, interface programs are provided for a fairly general class of models.

The software is written in Fortran 77, embedded in an Ansi-C environment (for the overall 'master program', which calls the various FORTRAN subprograms).

Examples of application include sensitivity analysis of a Model for Pesticide Leaching and Accumulation (Tiktak et al., 1994) and user subjectivity in MC modelling of pesticide exposure study (Beulke et al., 2006). An executable version of UNCSAM along with documentation is available from the RIVM.



## 2.16 UNCSIM

UNCSIM Systems analysis toolbox has been developed at EAWAG (The Swiss Federal Institute of Aquatic Science and Technology) to analyse the sensitivity of model results to model parameters, detect causes of (potential) identifiability problems of model parameters for a given measurement layout, and perform model predictions that include an estimate of their uncertainty (Reichert, 2006). The software interacts with an arbitrary simulation programme through a simple, text file based interface, independent of computing platform and programming language. UNCSIM provides elements required for a systems analysis toolbox to be used to calibrate, analyse and apply a model implemented in any simulation programme that supports the interface. The software supports maximum likelihood parameter estimation. The model parameters uncertainty propagation to the model is analysed using MC methodology. Sampling from a variety of multivariate distributions is supported (Reichert, 2005).

The tool is aimed at scientists working with frequentist and Bayesian inference of parameters of a simulation model. The examples of application include UNCSIM interfaces with process-based models, such as SWAT (Yang et al., 2007) and AQUASIM (Reichert, 2006). The program is available through <http://www.uncsim.eawag.ch/program/>.

## 2.17 UQLab

The UQLab project aims at the development of a MATLAB-based software framework for uncertainty quantification (Marelli and Sudret, 2014). It is designed to encourage both academic researchers and field engineers to use and develop advanced and innovative algorithms for uncertainty quantification, possibly exploiting modern distributed computing facilities. The tool code key features include extendibility and use of non-intrusive stochastic methods as Polynomial Chaos Expansion. It also includes an advanced Kriging toolbox. This modular platform comprises an optimized core probabilistic modelling engine and a simple programming interface that provides unified access to heterogeneous high performance computing resources. The tool provides a content-management system that allows users to easily develop additional custom modules within the framework.

The uncertainty quantification is allowed by data representation and sampling from complex multivariate distributions. The tool includes an extensive library of marginal distributions, modelling dependence with Gaussian copula, advanced sampling strategies (space-filling) like LHS and nested LHS, support for custom defined and bounded marginals and isoprobabilistic transform facilities. UQLab offers access to MATLAB-based models as well as a simple interface to connect third party modelling software for uncertainty propagation analysis (Lataniotis et al., 2015).

The software can be downloaded from: <http://www.uqlab.com/#!/download/c1kdf>.

## 2.18 R package ‘propagate’ and R packages referring to uncertainty estimation

### 2.18.1 ‘propagate’

The R package ‘propagate’ has been developed at the University of Hamburg (Spiess, 2015). The purpose of the package is to analyse propagation of uncertainties (“error propagation”) of inputs through an R expression (an object that represents an action that can be performed by R). The propagation function is a general function for the calculation of uncertainty propagation by first- and second-order Taylor expansion and MC simulation including covariances. Input data can be any symbolic/numeric differentiable expression and data based on replicates, summaries (mean and standard deviation) or sampled from a distribution. Uncertainty propagation is based on matrix calculus accounting for the full covariance structure. MC simulation is conducted using multivariate normal or t-distributions with covariance structure. The second-order Taylor approximation in ‘propagate’ uses a second-order polynomial to account for nonlinearities, making heavy use of numerical or symbolical Hessian matrices. The package supplies plotting functions, e.g. graphing error propagation with histograms of the MC simulations and MC/Taylor-based confidence intervals. The MC sampling can be realized for 15 continuous distributions.

There is no documented application of ‘propagate’ (Spiess, A., personal comm.). The package is available through CRAN.

### 2.18.2 Other R packages referring to uncertainty estimation

Many R packages available through CRAN cover some aspects of UQ within a specific scientific problem. There is also a number of packages that deal with sensitivity analysis, optimisation, MC and Bayesian analysis. Examples include:

- ‘FME’ (A Flexible Modelling Environment for Inverse Modelling, Sensitivity, Identifiability, MC Analysis) - provides functions to assist fitting models to data, to perform MC, sensitivity and identifiability analysis. It is intended to work with models that are defined through a set of differential equations and solved either by an integration routine from package `deSolve`, or a steady-state solver from package `rootSolve`. However, the methods can also be used with other types of functions (Soetaert and Petzoldt, 2010).
- ‘mcmcse’ (Monte Carlo Standard Errors for MCMC) - provides tools for computing MC standard errors (MCSE) in MCMC settings. MCSE computation for expectation and quantile estimators is supported as well as multivariate estimation. The package also provides functions for computing effective sample size and for plotting MC estimates versus sample size (Flegal et al., 2016).
- ‘ArArRedux’ (Rigorous Data Reduction and Error Propagation of Ar40 / Ar39 Data) - processes noble gas mass spectrometer data to determine the isotopic composition of argon (comprised of Ar36, Ar37, Ar38, Ar39 and Ar40) released from neutron-irradiated potassium-bearing minerals. It then uses these compositions to calculate precise and accurate geochronological ages for multiple samples as well as the covariances between them. Error propagation is done in matrix form, which jointly treats all samples and all isotopes simultaneously at every step of the data reduction process (Vermeesch, 2015).

- 'betaper' (Functions to incorporate taxonomic uncertainty on multivariate analyses of ecological data) - Permutation method to incorporate taxonomic uncertainty and some functions to assess its effects on parameters of some widely used multivariate methods in ecology (Cayuela and de la Cruz, 2012).
- 'BVS' (Bayesian Variant Selection: Bayesian Model Uncertainty Techniques for Genetic Association Studies) - The functions in this package focus on analysing case-control association studies involving a group of genetic variants. In particular, it addresses modelling the outcome variable as a function of a multivariate genetic profile using Bayesian model uncertainty and variable selection techniques (Quintana, 2012).
- 'decisionSupport' (Quantitative Support of Decision Making under Uncertainty) - Supporting the quantitative analysis of binary welfare based decision making processes using MC simulations. Decision support is given on two levels: (i) The actual decision level is to choose between two alternatives under probabilistic uncertainty. This package calculates the optimal decision based on maximizing expected welfare. (ii) The meta decision level is to allocate resources to reduce the uncertainty in the underlying decision problem (Luedeling and Göhring, 2016).
- 'UncerIn2' (Implements Models of Uncertainty into the Interpolation Functions) – Provides tools for basic (random) data, grids, six models of uncertainty, three automatic interpolations (idw, spline, kriging), variogram calculation and basic data visualization (Burian, 2015).
- 'usdm' (Uncertainty Analysis for Species Distribution Models) - This is a framework that aims to provide methods and tools for assessing the impact of different sources of uncertainties (e.g. positional uncertainty) on performance of species distribution models (Naimi, 2015)
- 'sensitivity' (Global Sensitivity Analysis of Model Outputs) - A collection of functions for factor screening, global sensitivity analysis and reliability sensitivity analysis. Most of the functions have to be applied on models with scalar output, but several functions support multi-dimensional outputs (Pujol et al., 2015).



### 3 Obj. 2: Overview of current and planned usage of UQ tools within QUICS project

Within the QUICS project the uncertainty quantification constitutes a core of research. Each fellow looks at specific aspects of uncertainty quantification in integrated catchment modelling. Table 2 gives an overview of the uncertainty aspects that are researched by each fellow and the software they chose to carry out their research.

Despite numerous platforms available to deal with UQ (Chapter 2), majority of QUICS fellows, with exception of two, chose to develop their own code for their analysis in R, MATLAB or Python. The remaining two fellows plan to use the code developed by others. The high level languages like R, MATLAB or Python are becoming increasingly popular within scientific community. The main QUICS fellows motivations for choosing those included:

- availability – open source and sharable code allow for flexibility in developing code and modifying existing one;
- familiarity – especially R and MATLAB are widely used in science higher education;
- compatibility – several projects within QUICS are based on precursory studies and involve software packages developed in one of these three languages;
- learning – the choice of implementation of UQ analysis methods, rather than using available UQ software allows the control over analysis, ability to manipulate it and test new methods.

Table 3 Overview of the software used for uncertainty quantification in the QUICS project.

Fellow	Project title	Aspect of uncertainty propagation	Chosen software/programming platform	Motivation
ESR1 - Carla Camargos	Landscapes as generators of water resources for urban areas, uncertainty of agriculture on water quality and quantity	SWAT model input and validation data uncertainty, model parameters and structure using DRAM (Delayed Rejection and Adaptive Metropolis) and Bayesian approach	Planning to use R scripts (SWAT-FME package/spup-package) and the Python package Spotpy	Selected packages are developed specifically for the SWAT model
ESR2 - Alexandre Wadoux	Sampling design optimisation for uncertainty propagation analysis	Model parameters uncertainties propagation analysis (via Bayesian calibration of the SWAT model)	R	Free, widely used, ability to employ existing code
ESR3 - Arturo Torres	Optimal complexity of urban sewer system models accounting for spatial uncertainty propagation across different scales	Analysing input uncertainty propagation through a simplified urban drainage model EmitStatR (MC approach)	Developing own scripts for Monte Carlo simulation and input uncertainty propagation and analysis in R	R is a well-known programming language in the statistical community and further development of packages in this domain contributes to the user community
ESR4 - Mahmood Mahmoodian	Model reduction analysis under uncertainty for a Multiple Model Predictive Control to dynamically manage water quality	Quantifying the overall uncertainty imposed by model reduction	MATLAB or Python	The study case is based on model reduction using MATLAB. Therefore, it is more handy and beneficial to have the uncertainty propagation tool in the same platform
ESR5 - Omar Wani	Assessing influence of model structure deficiencies and input errors on the uncertainty of model output, method development	Developing general UQ methodologies. Specifically developing the bias technique that incorporates input and model structure uncertainty, whereas model parameter uncertainty is captured in the posteriors of parameters after Bayesian inference	R	R is a good language for statistical analysis. It is free and has many packages already written in it (common knowledge)
ESR7 - Antonio Manuel Moreno Rodenas	Propagation of uncertainties in integrated urban drainage models	Assessing how uncertainties behave through a full scale integrated catchment model for Dissolved Oxygen Concentration predictions in a river. The aim is to separate data-wise sub-models to be able to perform an uncertainty propagation from the output of one towards the input of the next one	Python	Developing suit for controlling the WEST software from ironpython (WEST is a commercial modelling software which works under Tornado which is a .net software platform), therefore choosing Python for compability

Table 2 Continuation.

Fellow	Project title	Aspect of uncertainty propagation	Chosen software/programming platform	Motivation
ESR8 – Ambuj Sriwastawa	Uncertainty analysis frameworks linked to asset management decisions	Input data uncertainty propagation (using Markov Chain Monte Carlo Approach)	MATLAB, add-on tool developed at Aquafin, Belgium. R in the future.	The Aquafin tool allows automated simulations on InfoWorks CS. R is freely available and commonly used.
ESR9 - Vivian Camacho	Quantification of uncertainties associated with fluvial pollutant transport	Model structural uncertainty (by comparing several models (advection dispersion in 1D, 2D and 3D) to observed data from a specific river. Comparison of models to lab measurements, parameter uncertainty (MC analysis on the dispersion coefficients obtained from empirical equations for the case study and for the lab experiment), input uncertainty (MC and Bayesian analysis)	Developing own scripts in Python	Familiarity, developing own scripts is suitable to learn about the uncertainty analysis methods and also gives more flexibility about applying them
ESR10 - Francesca Cecinati	Propagation of rainfall radar uncertainties linked with water quality models	Looking at uncertainty estimation and propagation for radar data and models requiring rainfall as input data	Developing own software in MATLAB and R. Plan to use a toolbox for MATLAB developed in Bristol for uncertainty and sensitivity analysis (SAFE toolbox)	Developing own software allows for being aware of each passage, being able to manipulate it, modify it and come up with new methods. The SAFE toolbox is developed by colleagues here in Bristol, and it is worth to evaluate how it performs with given data
ESR11 - Mano Muthusamy	Effect of climate change and rainfall variability on urban sediment behaviour	Looking at input uncertainty propagation due to spatial upscaling of point rainfall data in urban sediment transport models (Lump catchment models)	R	Familiarity, free to use
ESR12 - Nazmul Beg	Uncertainty analysis of hydraulic structures behaviour, 2D & 3D to 1D	Looking at model input uncertainties (using turbulence models and Bayes approach)	R scripts developed by ESR5	R is a good language for statistical analysis. It is free and has many packages already written in it (common knowledge)
ER1 - Kasia Sawicka	Propagation Analysis Tools	Input data and model parameter uncertainty propagation to the model output	R	Free, includes advanced statistical and graphic capabilities, widespread in science and education
ER2 - Mathieu Lepot	Produce methods for data management under uncertainty	Looking at input uncertainties, model parameters and residuals. Developing a general methodology where Law of Propagation of Uncertainty and MC simulation are applied	Developing own code with MATLAB	Familiarity, widely used, code can be compiled as self-standing application for wider use

## 4 Obj. 3: Overview of the UQ tool (*spup* R package) developed at WU

### 4.1 Motivation

Advances in uncertainty propagation and assessment have been paralleled by a growing number of software tools for uncertainty analysis (Chapter 2 ). Nevertheless, none has gained recognition for a universal applicability, including case studies with spatial models and spatial model inputs. Due to the growing popularity and applicability of the open source R programming language WU has undertaken a project to develop an R package that facilitates uncertainty propagation analysis in spatial environmental modelling. The tool is intended for researchers and practitioners who understand the problems of uncertainty in data and models, and are looking for a simple, accessible implementation of the universal methodology for uncertainty assessment. At the same time, it is designed to enable more experienced users to easily understand, customise, and possibly further develop the code.

A number of computational tools are readily available to tackle the uncertainty quantification problem to different degrees (Chapter 2 ). To the best of our knowledge, however, none of the existing software has been widely acquired by the environmental science community for uncertainty propagation analysis. The use of powerful but complex languages like C++ (e.g. Dakota), Python (e.g. OpenTURNS) or Java (e.g. DUE) often discourages relevant portions of the non-highly-IT trained scientific community from the adoption of otherwise powerful tools.

The R programming language has become an important language for the development of numerical and statistical analysis tools. R has advantages through its advanced statistical capabilities and high-quality graphical output (Ripley, 2001), and is gaining widespread use in science and education. Furthermore, through the use of R packages, the software can be used for a variety of geoscience analyses and visualisations. It has grown tremendously over the last 20 years, with over 8000 packages at the time of preparation of this report. There is a number of R packages referring to the uncertainty analysis through sensitivity analysis or use of a Bayesian framework for model calibration. We have found only one package named 'propagate' (Section 2.18.1) that deals with uncertainty propagation explicitly, using similar approaches as described in the following of this report. The package 'propagate', however, does not provide functionality for spatial models and variables.

### 4.2 Employed (spatial) uncertainty propagation analysis approach

Uncertainty propagation aims to analyse how uncertainties in data (e.g. from measurement error, sampling, interpolation), combined with model uncertainties (e.g. in the model parameters and structure) propagate through the model (Heuvelink et al., 2007). Many environmental phenomena of interest are spatial, temporal or spatio-temporal in nature and often have strong correlations imposed by the physics and dynamics of the natural systems, making uncertainty evaluation difficult. The most frequently used approach represents uncertainty with pdfs. The pdf describes the likelihood of a random variable to obtain a given value, and typically it is viewed as the shape of the distribution, for example normal, uniform, lognormal or exponential. It is common for the pdf to be parameterized, i.e. to be characterized by distribution parameters. For example, the normal distribution is parametrized in terms of the mean and the variance, while the uniform distribution is parameterized by minimum and maximum values. For situations in which pdfs can be estimated

reliably, they have a number of advantages over non-probabilistic techniques. They include methods for describing cross- and auto- correlation between uncertainties, methods for propagating uncertainties through simple algebras or more complex environmental models, and methods for tracing the sources of uncertainty in environmental data and models (Heuvelink, 1998).

A frequently used method for the analysis of uncertainty propagation is the MC method (Hammersley and Handscomb, 1979, Lewis and Orav, 1989). It is very flexible and can reach an arbitrary level of accuracy, and therefore it is generally preferred over analytical methods such as the Taylor series method (Heuvelink, 1998). The idea of the MC method is to compute the output of the model repeatedly, with input values that are randomly sampled from their marginal or joint pdf. The set of model outputs forms a random sample from the output pdf, so that the parameters of the distribution, such as the mean, variance and quantiles, can be estimated from the sample. The method thus consists of the following steps:

1. Characterise uncertain model inputs with pdfs.
2. Repeatedly sample from (spatial) pdfs of uncertain inputs.
3. Run model with sampled inputs and store model outputs.
4. Compute summary statistics of model outputs.

Note that the above ignores uncertainty in model parameters and model structure, but these can easily be included if available as pdfs (such as obtained through Bayesian calibration). A random sample from the model inputs can be obtained using an appropriate pseudo-random number generator (Lewis and Orav, 1989). Note that a conditioning step will have to be included when the model inputs are correlated. Application of the MC method to uncertainty propagation with operations that involve spatial interactions requires the simultaneous generation of realisations from the spatially distributed inputs, implying that spatial correlation will have to be accounted for (Heuvelink et al., 1989). For uncertain spatially distributed continuous variables, such as elevation, rainfall and soil organic carbon content, we assume the following geostatistical model:

$$Z(x) = \mu(x) + \sigma(x) \cdot \varepsilon(x) \tag{1}$$

where  $\mu$  is the (deterministic) mean of the variable of interest  $Z$ ,  $\sigma$  is a spatially variable standard deviation associated with the prediction  $\mu$  (spatial variability of  $\sigma$  reflects that in some parts of study area the uncertainty is greater than in other parts), and  $\varepsilon$  is a standardized, zero-mean, spatially auto-correlated residual modelled with a semivariogram or a correlogram (Diggle and Ribeiro, 2007, Webster and Oliver, 2007, Plant, 2012). The random sample is drawn from the pdf of  $\varepsilon$  to further calculate the realizations of  $Z$ .

The drawback of the MC method is that the accuracy of the uncertainty assessment is inversely related to the square root of the number of runs  $N$ . This means that to double the accuracy, four times as many runs are needed. In complex, multi-variable systems high accuracies are obtained only when the number of runs is very large (i.e.  $N \geq 1,000$ ), which may cause the method to become extremely time consuming. The improvement on MC efficiency can be made by employing efficient sampling techniques (e.g. LHS) and parallel computing.

### 4.3 'spup' (spatial uncertainty propagation) package design

The adopted approach for uncertainty propagation analysis dictates the general package design. The 'spup' package provides functions for examining the uncertainty propagation starting from input data and model parameters, via the environmental model onto model outputs (Figure 10). The functions include uncertainty model specification, stochastic simulation and propagation of uncertainty using MC techniques, as well as several uncertainty visualization functions.

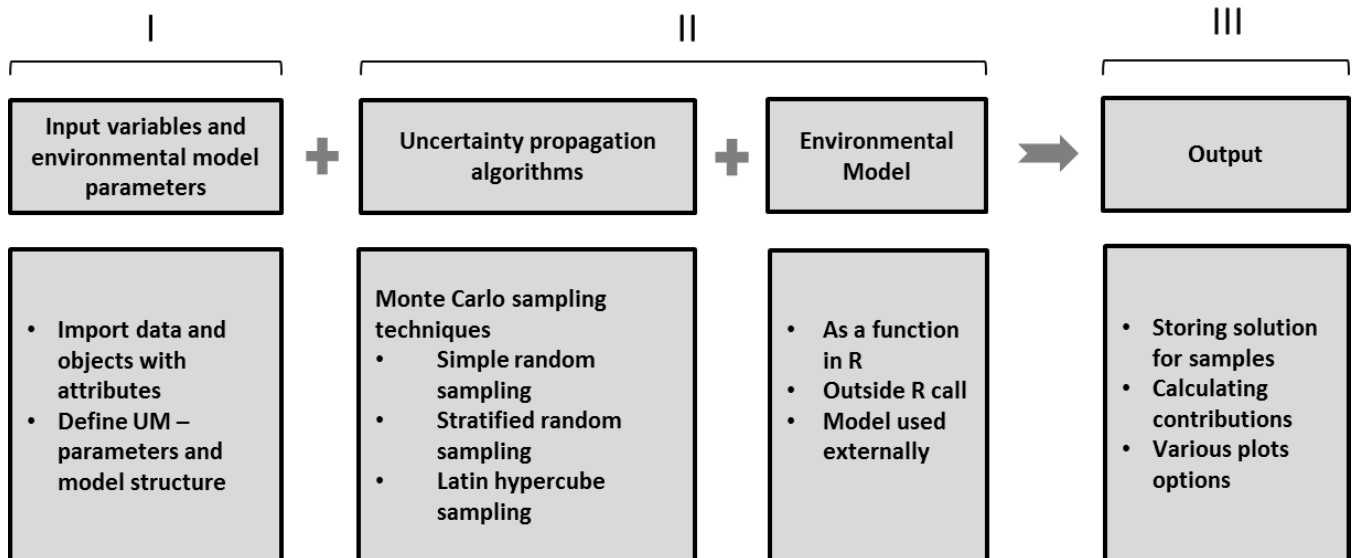


Figure 10 . The 'spup' package design. 'spup' comprises of functions for defining the uncertainty model (I), quantifying uncertainty propagation (II) and storing output in a format of data or images.

Uncertain environmental variables are represented in the package as objects whose attribute values may be uncertain and described by probability distributions. Uncertainty may also be ignored for some inputs, in which case, during the model run the user works with  $\mu$  (Eq. 1) as the model input that best represent the reality. Both numerical (e.g. air humidity) and categorical data (e.g. land cover) types are handled. Spatial auto-correlation within an attribute and cross-correlation between attributes is also accommodated for. The attributes may be independent in space, for which a marginal probability density function (mpdf) is defined at each point in space, or may co-vary in space, for which a joint probability density function (jpdf) is defined. Different shapes of marginal pdfs are supported, whereas joint pdfs may be defined for groups of attributes characterized with the normal distribution only. The specification of correlations between errors in space and cross-correlations between objects or attributes is made under the assumption that the correlations depend only on the distance between locations.

For spatially correlated variables the package relies on unconditional Gaussian simulation implemented in the 'gstat' package (Pebesma, 2004). For drawing realizations of uncertain variables without assumed correlations the package has implemented the MC approach with efficient sampling algorithms, i.e. stratified random sampling and Latin hypercube sampling. The design includes facilitation of parallel computing to speed up MC computation. The MC realizations for uncertainty propagation quantification may be used as an input to the environmental models called from R, or externally.

Selected static (adjacent maps and glyphs) and interactive visualization methods that are understandable by non-experts with limited background in statistics can be used to summarize and visualize uncertainty about the measured input, model parameters and output of the uncertainty propagation. Currently, the implementation of visualization functions consist of adjacent maps, glyphs and interactive application. The adjacent maps and glyphs are used for continuous variables. Both allow for displaying maps with information about the ensemble mean and standard deviation. Adjacent maps were also used for categorical data, displaying maps of the most probable class, as well as its associated probability. The interactive applications include a graphical user interface, which in addition to displaying the previously mentioned variables also allowed for comparison of joint uncertainties at multiple locations. The implementation of the visualisations was done via calls to the ‘ggplot2’ package. The interactive methods are implemented using the ‘shiny’ package allowing users to activate the visualisation of statistical descriptions of uncertainty through interaction with a plotted map.

#### 4.4 ‘spup’ application example – mapping soil moisture content for the Allier catchment

To maximise package accessibility and usability for the user, ‘spup’ will include vignettes containing tutorials and application examples. This section presents one such example.

As part of a research study in quantitative land evaluation, the World Food Studies (WOFOST) crop simulation model (van Diepen et al., 1989) was used to calculate potential crop yields for floodplain soils of the Allier river in the Limagne rift valley, central France. The moisture content at wilting point ( $\Theta_{wp}$ ) is an important input attribute for the WOFOST model. Because  $\Theta_{wp}$  varies considerably over the area in a way that is not linked directly with soil type, it was necessary to map its variation separately to see how moisture limitations affect the calculated crop yield.

Unfortunately, because  $\Theta_{wp}$  must be measured on samples in the laboratory, it is expensive and time-consuming to determine it for a sufficiently large number of data points for creating the prediction map by kriging. An alternative and cheaper way is to calculate  $\Theta_{wp}$  from other indicators which are cheaper to measure. Because the moisture content at wilting point is often strongly correlated with the moisture content at field capacity ( $\Theta_{fc}$ ) and the soil porosity ( $\Phi$ ), both of which can be measured more easily, it was decided to investigate how errors in measuring and mapping these would work through to a map of calculated  $\Theta_{wp}$ . Calculation of  $\Theta_{wp}$  can be done using a pedo-transfer function, which in this case takes the form of multiple linear regression:

$$\Theta'_{wp} = \beta_0 + \beta_1 \cdot \Theta_{fc} + \beta_2 \cdot \Phi + \delta \quad (2)$$

where  $\Theta'_{wp}$  denotes measured moisture content at wilting point,  $\beta_0$ ,  $\beta_1$ , and  $\beta_2$  are the regression coefficients and  $\delta$  denote residuals attributed to lack of model fit and measurement error. The regression coefficients were estimated using standard ordinary least squares regression, ignoring spatial correlation between the observations at the locations. The maps of  $\Theta_{fc}$  and  $\Phi$  were derived using co-kriging and accounted for spatial cross-correlation between  $\Theta_{fc}$  and  $\Phi$ . Each component on the right hand side of Eq. 2 is subject to uncertainty, which will propagate to uncertainty about

$\Theta_{wp}$ . Following the adopted MC approach, for each variable and parameter the uncertainty model was defined and 1000 MC samples were drawn. For the spatial variables a linear model of co-regionalization (Wackernagel, 2003) was fitted with the use of the 'gstat' package and possible realities were simulated. The joint pdf of the model parameters and structural error  $\delta$  was estimated using Bayesian calibration (Van Oijen et al., 2005) (note, this is not included in the 'spup' package) and a random sample was drawn from their joint posterior distribution. 1000 realizations of  $\Theta_{wp}$  were then calculated using Eq. 2 and summary statistics such as mean of prediction and standard deviation were derived.

If uncertainty analysis with WOFOST shows that the errors in  $\Theta_{wp}$  cause errors in the output of WOFOST that are unacceptably large, then the accuracy of the map of  $\Theta_{wp}$  would have to be improved. In order to decide how to proceed in such a situation, the contribution of each individual error source to the overall uncertainty in  $\Theta_{wp}$  was determined as well. Figure 11 presents the results and these show that both  $\Theta_{fc}$  and  $\Phi$ , rather than model parameters and model structural error, form the main source of uncertainty. Thus, the main source of error in  $\Theta_{wp}$  is the one associated with the kriging errors of  $\Theta_{fc}$  and  $\Phi$ .

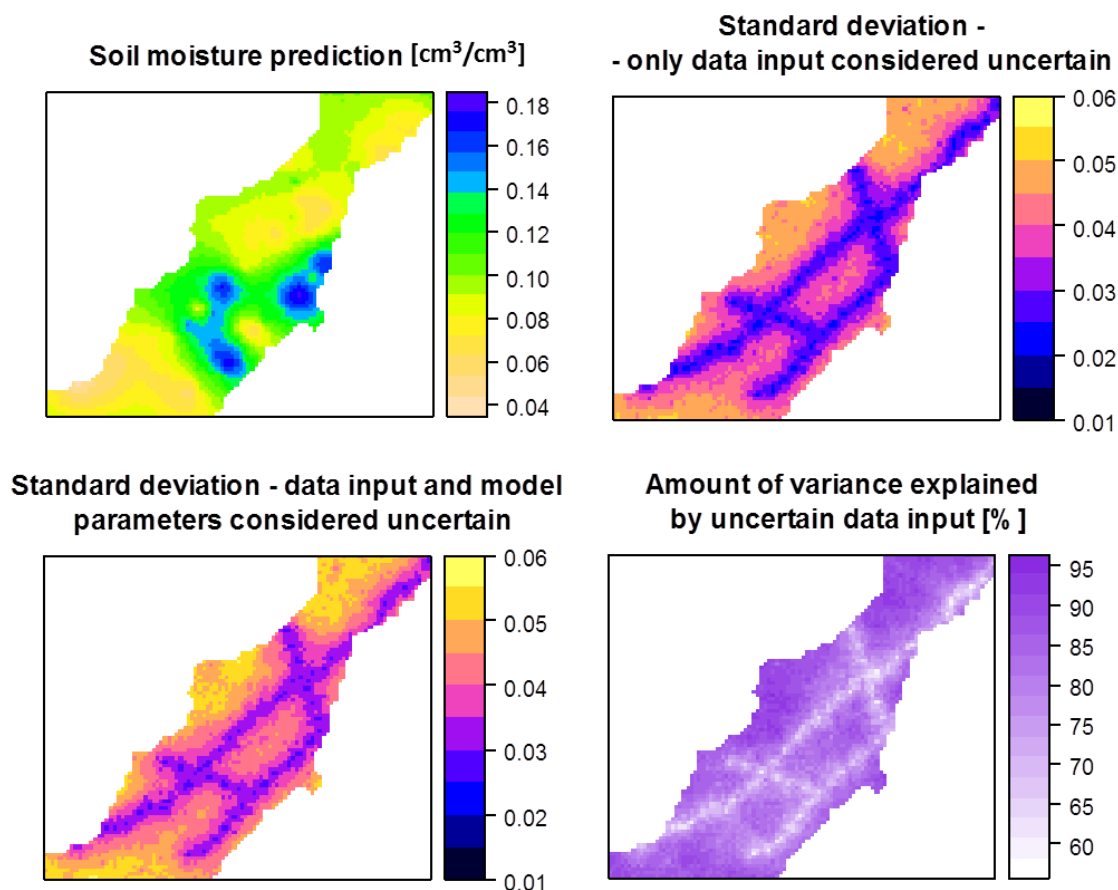


Figure 11 Results of uncertainty propagation for soil moisture prediction in the Allier catchment.



## 4.5 Further work on the 'spup' R package

As one of the contributions to the QUICS project and wider community it is aimed to develop a universal tool for uncertainty propagation assessment based on the uncertainty quantification framework described in e.g. Heuvelink et al. (2007). As the theoretical framework and implementation of the package progress, its application to real cases will be necessary, to test the algorithms and usability of the tool, demonstrate the importance of assessing uncertainty in environmental data, and provide tutorials for the users. As part of the collaborative work within QUICS, the potential case studies for the 'spup' application include uncertainty propagation analysis with the LandscapeDNDC model (Haas et al., 2012) and German Schwingbach catchment data, and Metaldehyde Prediction model developed currently for the Severn Trent Water, water provider in the Midlands, UK. Finally, 'spup' will be introduced to the wider scientific community through CRAN (The Comprehensive R Archive Network), where many more challenges will be faced, including the time and resources required to implement an uncertainty assessment and the need to make uncertainty analyses understandable to non-statisticians. The current progress has been presented at the EGU 2016 conference and is going to be presented at the Spatial Accuracy 2016 conference. The package is aimed to be published on CRAN in December 2016.

## 5 Conclusions

In this report a total of 18 software tools were identified to deal with uncertainty analysis, parameter estimation or sensitivity analysis. All of the identified tools are model-independent and can, in principle, be applied to evaluating any environmental model or modelling system. However, tool interoperability and comparison is complicated by the use of different coding languages, input-output formats, and approaches to execution management.

The assembled list of tools contains a considerable amount of overlapping functionality. This redundancy confounds practitioners tasked with selecting the best tool for the job. Unfortunately, recommending specific tools from the list is beyond the scope of this work, since they were not tested or exercised. In this context, it may be more useful to prioritize the underlying methodologies, as opposed to actual technology implementations. Ideally, uncertainty propagation analysis activities performed for decision support should include (1) data uncertainty propagation, (2) model parameter uncertainty propagation (3) model structure uncertainty propagation (4) contributions for propagated uncertainty, and (5) summary and visualization tools to identify areas that may be improved. The selection of software may depend on the researched aspect of this framework, however considering any single source of uncertainty (i.e. structural, parameter, and data errors) may lead to misleading uncertainty predictions in the model output: it is therefore important to consider all types of errors in a comprehensive, explicit and cohesive way to reduce bias and uncertainty in the final prediction.

Looking to the future of integrated environmental modelling, it is worth noting that high level languages (e.g., R, Python and MATLAB ) are becoming increasingly popular delivery mechanisms for uncertainty quantification tools and environmental models. Frameworks that can easily accommodate such languages will have an edge over those that only support lower-level languages (e.g., FORTRAN, C/C++, and Java).

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