NEURAL NETWORK APPROACH TO RESPONSE SURFACE METHODOLOGY IMPLEMENTED IN ALLIANCES

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The paper presents a simple test to illustrate the neural network approach in building a surface response using the Alliances platform. Alliances is a French numerical platform that allows simulation of all the phenomena governing the safety of nuclear waste storage and disposal.

The test presented simulates water flow in a porous media composed by two geological formations that represent the first two soil layers of the Saligny site that is the destination for the low and intermediate level waste repository in Romania. The test represents a modeling activity needed for the creation of the surface response in the simulation of the transport for the radionuclides with potential to be released from the repository. In order to obtain the surface response, input parameters related to the description of the soil layers (density, porosity, suction, soil water permeability, saturation) on site should be varied in their range. The test presented in this paper uses the real characteristics of the first soil layers from the Saligny site and vary only the permeabilities and the targeted output function is the water saturation of the geological media involved.

The output data predicted with the neural network based on the surface response methodology are obtained much faster than by running the model with the input variables of interest, making it a very attractive option when large domains of input parameters are investigated and running the model is very time costly.

Keywords: Alliances, NSRAWD, neural network, surface response

1. Introduction

The paper presents a simple test to illustrate the neural network approach in order to build a surface response using the Alliances platform, one of the modeling activities performed in the framework of the NSRWAD project (Numerical Simulations for Radioactive Waste Disposal) which proposed to establish a collaboration between the Institute for Nuclear Research (INR) and the French Alternative Energies and Atomic Energy Commission (CEA) in the field of numerical simulations for waste disposal. Alliances is a numerical platform that allows simulation of all the phenomena governing the safety of nuclear waste

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storage and disposal targeting efficient coupling of different numerical codes, simulation of complex physical and multi-scale phenomena, as well as uncertainty analysis of data and models.

The French Alternative Energies and Atomic Energy Commission (CEA) and the French Agency for Radioactive Waste Management (ANDRA) have been jointly developing since 2001 the software platform. Beginning with 2003, the French Electricity Company (EDF) brings its contribution to the project. The purpose of the project was to obtain a numerical platform to allow simulation of all the phenomena governing the safety of nuclear waste storage and disposal targeting efficient coupling of different numerical codes, simulation of complex physical and multi-scale phenomena, as well as uncertainty analysis of data and models.

During the NSRAWD project (2010-2013), several modeling activities concerning water flow and solute transport in porous media were performed targeting the creation of a surface response with Alliances for the contaminant transport in the unsaturated area of the Saligny site.

The studies performed so far to find a suitable host for a low and intermediate level waste repository in Romania have indicated the Saligny area as a convenient option due to its main advantages such as the immediate neighborhood with the nuclear power plant from Cernavodã and its dry climate. In the present, the status of this option is close to certitude and efforts are made constantly in order to implement the disposal facility.

The unsaturated area refers to a fairly thin zone of a few to several tens of meters, above the groundwater table, where part of the pore space is occupied by the air phase.

The final purpose of the activities performed in the framework of the NSRAWD project may be an integrated system for the safety assessment of low and intermediate level waste disposal applied to the Saligny site as an useful method for the future licensing applications of the disposal sites. Surface response for the transport of the radionuclides (that have potential to be released from the repository) through geological media surrounding the repository is needed to build this integrated system.

In order to obtain the surface response, input parameters related to the description of the soil layers (density, porosity, suction, soil water permeability, saturation) on site should be varied in their range. The variation of the input parameters describing the soil layers were previously determined in a characterization national program for the Saligny [**i**] site based on large amounts of samples collected from drillings performed on site.

The test presented in this paper uses the real characteristics of the first soil layers from the Saligny site (layer width, porosity, residual water content, permeability, van Genuchten parameters that describe the soil water retention characteristics) and vary only the permeabilities and the targeted output function is the water saturation of the geological media involved. Deterministic input parameters for the soil layer (porosity, layer width) were taken from the mediation of experimental data available for the first two layers [**i**] and residual water content, θ_r as well as the van Genuchten parameters were inferred from fitting the computed water saturation profile on measured profile on site. The work performed in order to obtain θ_r and the van Genuchten parameters is described in detail in [**ii, iii, iv]**. The range of soil permeability was established from minimum and maximum measured value for each layer and the distribution was considered uniform for simplicity and for test purpose.

Modeling of water flow and contaminant transport in the unsaturated area of the Saligny site accomplished in the framework of the NSRAWD project was described in [**v**, **vi**]. NSRAWD project will continue with NSRAWD2 project (2014-2016) that will target to develop starting from the test presented and the variation of the input parameters the surface response for contaminant transport in the unsaturated area of the Saligny site.

2. Neural network approach and Alliances

An artificial neural network is a distributed system for parallel processing of information (software and/or hardware) composed of finite non-linear processing elements called artificial neurons that are interconnected based on a given topology and giving the ability to quantitatively modify the values assigned to connections and the processing parameters. Basic concepts of the neural network, their architectures and algorithms are presented in [**vii**, **viii**, **ix**, **x**].

Response surface methodology (RSM) is a collection of mathematical and statistical techniques for empirical model building. By careful design of *experiments*, the objective is to optimize/ analyze a *response* (output variable), y which is influenced by several *independent variables* (input variables), $x_1, x_2, \ldots,$ x_k [**xi**]. In general, the relationship between response and the input variables is unknown but can be approximated by a low-degree polynomial model of the form:

$$y = f'(x)\beta + \varepsilon \tag{2.1}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_k)$_, $f'(x)$ is a vector function of p elements that consists of powers and cross-products of powers of $x_1, x_2, \ldots, x_k$ up to a certain degree denoted by d (≥ 1), β is a vector of p unknown constant coefficients referred to as parameters, and ε is a random experimental error assumed to have a zero mean [**xii**].

Two important models are commonly used in RSM [**xii**]. These are special cases of model (3.3.1) and include the first-degree model ($d = 1$),

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \varepsilon \tag{2.2}$$

and the second-degree model (d = 2),

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i<j}\sum \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon \tag{2.3}$$

Originally, RSM was developed to model experimental responses, and then migrated into the modelling of numerical experiments. The difference is in the type of error generated by the response. In physical experiments, inaccuracy can be due, for example, to measurement errors while, in computer experiments, numerical noise is a result of incomplete convergence of iterative processes, round-off errors or the discrete representation of continuous physical phenomena. In RSM, the errors are assumed to be random [**xi**].

The application of RSM to design optimization is aimed at reducing the cost of expensive analysis methods (e.g. finite element method or CFD analysis) and their associated numerical noise, providing in the same time:

- a way to establish a relationship, albeit approximate, between y and $x_1, x_2, \ldots, x_k$ that can be used to predict response values for given settings of the control variables;
- determination, through hypothesis testing, of the significance of the factors whose levels are represented by $x_1, x_2, \ldots, x_k$;
- determination of the optimum setting for $x_1, x_2, \ldots, x_k$ that results in a maximum/minimum response over a certain region of interest.

In order to achieve these objectives, a series of *n* experiments (called *runs*) should first be carried out, in each of which the response *y* is measured (or observed) for specified settings of the control variables. The totality of these settings constitutes the so-called response surface design [**xi**]. A good design for numerical experiments should give a maximum of effects with a minimum of computed points as well as should be well balanced among the set of values of the input variables. Latin Hypercube Sampling (LHS) satisfies both of these assertions.

An illustrative example for using the RSM methodology in solute transport modeling may be the following application: the transport of a contaminant by the infiltration of water introduced through a point source in a 2D unsaturated porous media, having imposed boundary conditions on pressure. The aim is to study the values of the van Genuchten α parameters from the saturation law as well as the values of the dispersivity coefficients that maximize the concentration of contaminant in a specified point of the domain investigated, at a certain moment of time.

The response can be represented graphically, either in the three-dimensional space or as *contour plots* that help visualize the shape of the response surface. Contours

are curves of constant response drawn in the x_i, x_j plane keeping all other variables fixed. Each contour corresponds to a particular height of the response surface.
The effective working methodology with Alliances platform requires installation of an additional module called Uranie and assumes several steps in which support Python scripts are created and run in a certain order to obtain in the end the data file that constitutes the surface response. First the experimental design is established as well as the range of input variables. In order to build an approximation model able to capture the interactions between the k design variables, a sampling technique is required for the investigation of all significant combinations of input parameters in their ranges imposed. Among the most known sampling methods are the full factorial approach, the central composite approach, the D-optimal approach and the Latin hypercube approach. Although several sampling methods are implemented in Alliances, Latin hypercube sampling remains the recommended option. After sampling is done, the computer code (e.g. the transport model) is launched several times for each of the data sets obtained from sampling. An example database is subsequently created, composed of sets of input variable and their responses. A learning database which is a subset of the example database is also created and it is used to build the neural network. A testing database, another subset of the example database, is used to validate the neural network based on the mean square criteria. The output data predicted with the neural network based on the surface response methodology are obtained much faster than by running the model with the input variables of interest.

3. Example test to illustrate neural network approach in Alliances

The test considered is a water flow steady state problem in a 1D vertical (along z coordinate) two layers porous system illustrated in Fig. 1.

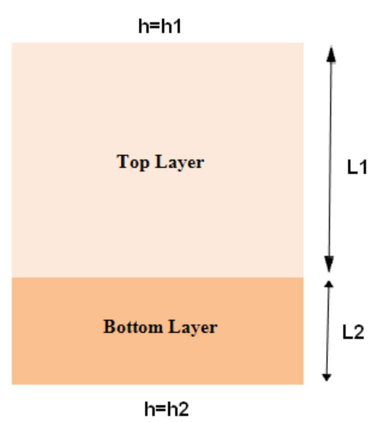

Fig. 1 Test case geometry

A comprehensive presentation on the fundamentals of water flow in porous media can be found in [**xiii**]. The description of the water flow computation in Alliances is accomplished in [**xiv]**. The comparison between the computer simulation performed with Alliances and the analytical solution of this simple test is presented in [**xv**].

The boundary conditions at the top and the bottom of the system are of Dirichlet type.

Imposed boundary conditions are depicted in **Fig. 1**. The initial conditions are defined through an initial constant saturation inside each layer which is equivalent through saturation – pressure relationship to an initial constant pressure h in each soil layer. Numerical values defining initial and boundary conditions are presented in Table 1:

Table 1

Initial and boundary conditions

Conditions	**Top Layer**		**Bottom Layer**	
	h [m]	S_{eff} [-]	h [m]	S_{eff} [-]
Boundary	-6.2162	0.4	-2.9615	0.7
Initial	-4.1640	0.5	-1.5733	0.8

The system described in **Fig. 1** is discretized in space using 10 cells for the top layer and 5 cells for the bottom layer (each cell is then 1 m long). The resulting mesh of the system is then made of 15 parallelipiped cells. The problem considered is steady state, even though, we consider and computed a transient one until a final date of t_f=100 years (considered large enough to obtain a steady state) using a constant time step of δt = 1 year.

In steady state, the governing equations for water flow in porous media with variable saturation is described by the following equations:

$$div(K(h)\cdot grad(h+z))=0 \tag{3.1}$$

$$S_{eff}=\left(1+\left(\alpha\cdot|h|\right)^{n}\right)^{-m} \tag{3.2}$$

$$K(S_{eff})=K_0 S_{eff}{}^{3} \tag{3.3}$$

where K is the water permeability [m/s], S_{eff} is the effective saturation, h is the pressure head [m], z is the elevation [m] and α, m and n are the van Genuchten parameters from the soil water retention curve. The functions given for effective saturation is of van Genuchten type and the permeability law considered is cubic.

The target output was saturation in a certain point (having coordinates (0.5, 4)), arbitrary chosen in the Bottom Layer such as to obtain a function of the permeabilities of both layers considered. The input variables were the water permeabilities of the two layers. An uniform distribution of the permeability

values was considered for both layers in the variation interest range of the permeability parameter. Latin Hypercube approach was used for sampling.
The procedure implemented in order to use the capabilities of the Uranie module for computing water flow in porous media for this simple example is presented below:

(1) create the Python script for deterministic case (HF.py)
(2) sampling the input data through some specialized objects and classes available in Alliances; the result is put in a text file named „samplealt.dat”. A number of 100 value is considered at this step, for the test case considered. The Python code written is the following:

```
from sensitivity import *
# permeability of top layer
 minKTL=6E-7
 maxKTL=8E-7
# permeability of bottom layer
 minKBL=7E-8
 maxKBL=9E-8
# cf sensit_variable.py
KTL  = StochasticData('KTL' , Uniform(minKTL,maxKTL))
KBL  = StochasticData('KBL', Uniform(minKBL,maxKBL))
sample = Sample([KTL, KBL], 'LHS')
exp = Sampling(100,15032002, [sample])
exp.run()
exp.save('samplealt.dat')
```

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(3) adding the input variable of interest in a Python dictionary
(4) launching the test case using the sampling data and the result data is appended as a new column in the sampling data table; a new data file is created (i.e. result_sample.tab) which represents the example database. At this step, the code is run for each of the 100 values determined in (2). The more complex is the code, the more time consuming is the computation.

```
import os, sys            # for file path
from datamodel import *    # common model for all Alliances Data
sample_file='samplealt.dat'
import subprocess
table=makeTableFromFile(sample_file)
nr = table.getNbRows()
script = 'HF.py'
print nr
f=open('launch.log','wb')
for i in range(nr):
    row = table.getRow(i)
    print '%.13f %.13f'%(row[0],row[1])
    subprocess.call(["python",script,"--KTL=%.13f"%(row[0]),"--
KBL=%.13f"%(row[1])],stdout=f,stderr=f)
```

```
  pass
result_file='saturation_point.tab'
sampletab = makeTableFromFile(sample_file)
resulttab = makeTableFromFile(result_file)
column = resulttab.getColumn(0)
sampletab.addColumn('(0.5,4)',column)
sampletab.writeToFile('result_sample.tab')
```

----

(5) a script similar to the one in step (2) is launched to build a larger amount of input datas to use the neural network with.

(6) building the neural network given the example database table (result_sample.tab). The neural network can be used to generate output data given the input datas generated previously.

```
from time import time
from metamodel import *
from tables import *
import getopt
import sys
tinitial = time()
nn=[20,30]
# Definition of a Neural object
mod=Neural(   nbIter=5,
              nbInitMat=2,
              sampleBasis=0.80,
              export='c++',
              neuralNumber=nn,
              tolerance=[0.00001],
              normalize='CR')
tab_appr = makeTableFromFile('result_sample.tab')
input=['KTL','KBL']
output=['s_05_4']
# Definition of a MetaModel object
meta=MetaModel(name='sensi',
              title='sensi',
              sample=tab_appr,
              input=input,
              output=output,
              method=mod,
              debug=1)
LearnError,testError=meta.run()
print LearnError
print testError
```

This procedure created for the simple test can be easily adapted to much more complex cases with more input variables of interest, the only impediment being the increasing power of computational resources needed as well as increasing computation time for step (2).

Fig. 2 presents the model data, the set of initial and boundary conditions, the input variables used for building the experimental design database and the response targeted for the simple test considered.

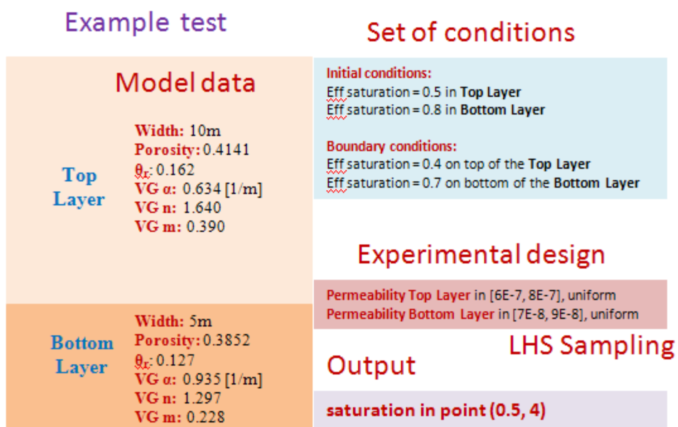

Fig. 2 *Response surface methodology implemented in Alliances for a simple example*

Fig. 3 presents the response surface for saturation in the chosen output point with coordinates (0.5, 4) having as input variables the permeabilities of the two soil layers of the system considered.

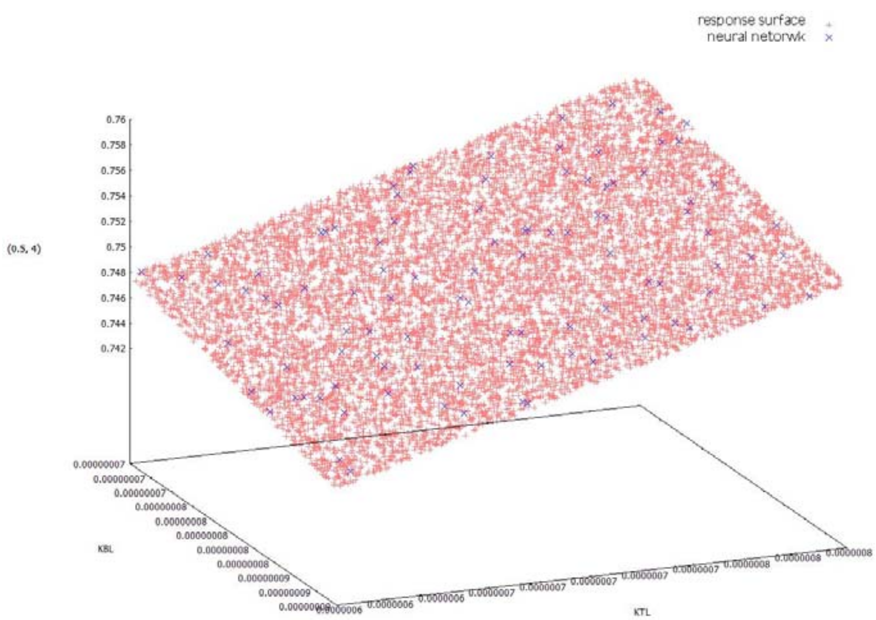

Fig. 3 Response surface for the example test

The computation time for obtaining the 100 neural network points in blue, by running the unsaturated flow model, is about 30 minutes whereas the time needed for obtaining the 10000 response surface points in red was only 2s.
The dependence of the output saturation point of the two input variables considered i.e. permeabilities of the two soil layers is represented as a plane surface, given the permeability law described by equation (3.3). The saturation in the specified output point (located in the bottom layer) increase with increasing the permeability of the top layer and decreasing the permeability of bottom layer.

It is to remind that the permeability describe the general ability of a geologic environment to transmit water. The computation result may be then expected as while the water permeability of the top layer is increased, the flow of water through the bottom layer is facilitated and, on the other hand, as the permeability of the bottom layer is decreased, the more water is retained in the bottom layer enabling a higher saturation of this media.

However, the interest of this simple test case created consists rather in preparing a procedure, based on the capabilities of Uranie module to deal with neural network, for a much more complex application where all the geological layers of the unsaturated zone of the Saligny site, together with the input parameters associated, as well as a contaminant transport instead of water flow computation should be addresed. The final objective for creating the surface response for contaminant transport in unsaturated area may be reached in this way. Once the computational procedure and tools are available, the remaining limitative issues consist in the time cost and computational resources needed. The more input parameters considered, the more computational memory is required. Investigating the capability to build the surface response for the contaminant transport in unsaturated area of the Saligny site was first addressed in the NSRAWD project and is proposed to continue in the NSRAWD2 project which is expected to start at the end of 2014. Distribution functions for porosity and water permeabilities for each of the seven layers composing the unsaturated zone of the Saligny site are already available based on experimental data [xvi]. The multitude of input parameters involved in such an analysis will make difficult the interpretation of results when dependence relationship, like the one obtained in the case presented, is no longer possible to be represented in the form of a surface. Contour plot representation approach is proposed together with a synthetic preview of a results in the form of minimum and maximum concentration of contaminant expected at the bottom of the unsaturated area of the Saligny site. The maximum concentration value is of great interest as, in the safety case needed in order to obtain construction licence for the final waste repository, it is converted in dose that may be received by a human receptor using water and food from the neighborhood of the repository.

4. Conclusions

The example test presented in this paper is meant to illustrate the way neural network approach is implemented in Alliances in order to build a surface response, starting with the well defined concepts of the neural network theory and following some basic steps to write the Python scripts needed to produce the expected results. The NSRWAD project in which this simple application was created proposed to explore and benefit from the capabilities of the Uranie module integrated in Alliances to further develop a surface response for the entire unsaturated area of the Saligny site. The purpose is to produce an integrated system for the safety assessment of low and intermediate level waste disposal applied to the Saligny site as an useful method for the future licensing applications of the disposal sites. The simple test is based on real parameters measured on two of the soil layers entering in the structure of the unsaturated area of the Saligny site and is a starting point for the more complex application targeted.

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