Feasibility of neural network metamodels for emulation and sensitivity analysis of radionuclide transport models

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Presenter: Kuan-Wen Liu
Advisor: Prof. Jui-Sheng Chen
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Abstract

This study explores the feasibility of using convolutional neural network (CNN) metamodels to emulate and analyze radionuclide transport models, with a focus on cesium-137 (137Cs) transport in sand. Traditional partial differential equation (PDE) models have been widely employed for simulating radionuclide transport; however, these models are computationally intensive and time-consuming, especially when applied to sensitivity analyses involving large parameter sets. By training CNNs on simulation outputs from PDE models, this research demonstrates that CNN metamodels can achieve high emulation accuracy with training sets of 40,960 samples or more. Sensitivity analyses performed using Sobol's first and total order methods reveal that CNN metamodels produce results comparable to those from PDE models while achieving significant computational speedup. Specifically, solving the PDE model for 10,240 realizations took 235 minutes, whereas the CNN metamodel completed the same task in just 3.5 minutes.

The study also investigates the impact of parameter tolerances on sensitivity indices, finding that CNNs are less affected by variations in parameter ranges than PDE models. The findings highlight the potential of CNN metamodels as computationally efficient alternatives to traditional PDE models, particularly for applications requiring large-scale simulations or real-time decision-making. This research provides a promising pathway for integrating deep learning techniques into environmental modeling to enhance computational efficiency without compromising accuracy.

Keywords: Convolutional Neural Networks (CNNs), Radionuclide, Sobol, Fipy.

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Jari Turunen & Tarmo Lipping

In this paper we compare the outputs of neural network metamodels with numerical solutions of differential equation models in modeling cesium-137 transportation in sand. Convolutional neural networks (CNNs) were trained with differential equation simulation results. Training sets of various sizes (from 5120 to 163,840) were used. First order and total order Sobol methods were applied to both models in order to test the feasibility of neural network metamodels for sensitivity analysis of a radionuclide transport model. Convolutional neural networks were found to be capable of emulating the differential equation models with high accuracy when the training set size was 40,960 or higher. Neural network metamodels also gave similar results compared with the numerical solutions of the partial differential equation model in sensitivity analysis.

Since decommissioning of the Hanford plutonium production site in the U.S state of Washington, the site has been under an active monitoring and remediation program to reduce the risks of radioactive contamination of the surrounding area[1,2]. Nuclear liquid waste in the Hanford area was stored originally in buried single-wall steel tanks containing NaCl and NaOH solution[1]. This dangerous waste material is currently being transferred to newly-built double-wall tanks; plutonium production waste leakage into the ground and especially into the Columbia River is being monitored annually[3,4].

When assessing the risk of contamination in Hanford, this leakage event can be compared to the Chernobyl incident in 1986, after which cesium (Cs) and strontium (Sr) radionuclides have been extensively studied. For example, doses of airborne ^{137}Cs and ^{90}Sr in food were monitored for over a decade in Romania. Peak values of 408.5 Bq/day of ^{137}Cs and 1.48 Bq/day of ^{90}Sr were measured in May 1986 from human food in[5]. Similar measurements were obtained in the Czech Republic where consumer milk was monitored for over a decade for ^{137}Cs and ^{90}Sr. Peak values of 506 Bq/l for ^{137}Cs and of 0.1 Bq/l for ^{90}Sr were obtained in 1986 in one of the samples[6]. In both cases, the ^{137}Cs doses were more than two orders of magnitude greater than the ^{90}Sr doses.

Despite the fact that the Chernobyl accident released both ^{137}Cs and ^{90}Sr[7] and the nuclear waste in Hanford contains approximately 24% of ^{137}Cs and 75% of ^{90}Sr[1], ^{137}Cs is the major concern in many studies concerning radionuclide contamination. The main reasons for this might be that ^{137}Cs bonds easily with chlorines to make salts, moves easily in the air, and dissolves easily in water[8]. ^{90}Sr is not transported as easily as ^{137}Cs, but plants growing in contaminated soil can take up small doses of both ^{90}Sr and ^{137}Cs[8,9]. In numerical simulations of groundwater, such as in[10,11], ^{90}Sr and ^{137}Cs mainly decay in the transportation phase, while part of the ^{90}Sr dose will stay in deep sediments and a fraction of both radionuclides could contaminate plants and animals. For example, ^{137}Cs tends to be absorbed by mushrooms, while ^{90}Sr tends to be spread to agricultural vegetables[11].

Due to the easy dissolution of ^{137}Cs in groundwater, the sediments in particular in Hanford may pose a threat to nearby residents. For that reason numerical simulations to determine the relation between transportation and absorption in sediments is essential. For example, Saiers et al. and Flury et al. have modeled the groundwater movement in Hanford sediments[12,13]. Both studies developed a partial differential equation (PDE) system fitted to the Hanford data. The results in both cases appear useful in making a numerical evaluation of cesium transportation and absorption in Hanford sediments.

Sometimes differential equation models are difficult to determine for some radionuclide interactions in the environment and very time consuming to solve. However, there are ways to address these problems. Reactive Transport Models (RTM) are one attempt to generalize sparse in-situ point data to cover the whole area to be investigated, while keeping the physical properties of the environment as accurate as possible. This can be done,

Tampere University, Pori 28100, Finland. email: jari.turunen@tuni.fi