MOBILITY MISSION REPORT

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MISSION TITLE

Meta-model for the homogenization of fractured porous media properties

DESCRIPTION

Concerned organisations

- Research entities
  - SCK CEN (Belgium)
  - Technical University of Liberec (Czech Republic)

Concerned infrastructures or facilities

- High-performance computing

Concerned phases

- Phase 1: Site evaluation and site selection
- Phase 2: Site characterisation

Themes and topics

- Theme 7: Performance assessment, safety case development, and safety analyses
    - Treatment of uncertainties

Keywords

fractured porous medium upscaling; homogenization of effective tensor of hydraulic conductivity; neural networks for upscaling; Multilevel Monte Carlo method

EXECUTIVE SUMMARY

Modelling groundwater processes is an important part of research on deep geological repositories of radioactive waste. As modelled processes involve uncertainties, we utilise the multilevel Monte Carlo method (MLMC) to obtain chosen statistics. However, MLMC cannot be applied directly when dealing with discrete fracture-matrix (DFM) models where both continuum and fractures are captured. In order to represent small fractures of a fine DFM model in a coarse DFM model, numerical homogenization is adopted. The numerical homogenization procedure is relatively slow because of the necessity of calling simulation software multiple times per MLMC sample. We investigated to what extent replacing numerical homogenization by a computationally-fast meta-model based on deep learning techniques, convolutional neural networks (CNN) in particular, can accelerate the MLMC computations.

During the mobility action, a meta-model for numerical homogenisation of the effective tensor of hydraulic conductivity of a DFM model was investigated. The specific architecture of deep neural networks that consists of a convolutional neural network followed by a feed-forward neural network was identified as a suitable meta-model to substitute original numerical homogenisation. The meta-model reaches an accuracy (R-squared) of ca. 90 % for all three independent values of hydraulic conductivity tensor.

Code integrating the existing mlmc library (Březina & Špetlík, 2022) and numerical homogenisation was developed. Employing the meta-model of numerical homogenisation within MLMC provides us with computational cost savings of around 50 % compared to MLMC using numerical homogenisation. The comparison was performed on a DFM model that simulates the effective tensor of hydraulic conductivity of the whole domain of interest. So far, only the two-dimensional case has been studied.

1. MISSION BACKGROUND

The future deep geological repository for radioactive waste in the Czech Republic is planned to be built on a crystalline rock. This type of rock is characterised by a negligible intergranular pore space. Groundwater flows predominantly through a fracture network in the rock. Despite all protective layers, stored radioactive waste will be exposed to the geosphere in the distant future and groundwater may become contaminated. This has motivated our aim to investigate groundwater processes as discrete fracture-matrix (DFM) models that consist of a continuum and a discrete fracture network. Although it is not feasible to measure all necessary properties of the rock environment, we know at least some of their statistics to consider them as random variables. In particular, the input to stochastic DFM models consists of spatially correlated random fields (SRFs) and a set of fractures with random properties. The modelling itself performs the Flow123d simulator (Březina et al., 2011).

1.1. R&D background

Monte Carlo methods might be adopted to obtain estimates of the expectation of some quantity of interest (QoI) resulting from a DFM model. The standard Monte Carlo method (MC) has a distinct drawback. Many runs of a highly accurate model must be performed to improve the accuracy of estimates. Consequently, the total computational cost of MC might be enormous. The multilevel Monte Carlo method (MLMC) (Giles, 2015) was developed to reduce the cost of MC. Unlike MC, MLMC does not run a single model repeatedly. Instead, a hierarchy of less accurate models approximates the same QoI as the original model but with a lower computational cost. Many samples are collected for less accurate models, while much fewer are collected for highly accurate models. The accuracy of a model is driven by the number of computational mesh elements.

Using MLMC for DFM models is a new challenging task. Considering a continuum model without fractures, small-scale mesh elements can easily be coarsened into a large-scale model. Regarding the continuum-fracture model, small fractures are beyond the resolution of large-scale models, but their impact cannot be neglected. Numerical homogenisation is employed to determine equivalent properties (e.g., hydraulic conductivity) from DFM models. Since sufficiently accurate MLMC estimates might require thousands of model realisations and the homogenisation procedure has to be performed many times, a meta-model of an original expensive model is used to accelerate calculations and make the whole procedure possible.

1.2. Mission objectives

The main scientific goal of the mobility action was to find a sufficiently accurate and computationally efficient meta-model for the numerical homogenisation process. In particular, we aimed to design a meta-model to determine the effective tensor of hydraulic conductivity of a DFM model and then use this meta-model as a part of the Multilevel Monte Carlo method. There is a wide range of meta-model design techniques. This mobility focused on neural networks. There are two main ideas. First, we aim to use rasterized SRF with fractures to train CNN to predict three independent elements of the effective tensor. The second approach consists in designing a hierarchical neural network of small CNNs. The latter might benefit from the inclusion of geometric parameters of fractures. Eventually, proposed approaches, designed meta-models, and achieved results will be published.

1.3. Mission request

To deepen knowledge of meta-models design techniques based on deep neural networks with an emphasis on convolutional neural networks.

To learn technologies used for machine learning at SCK CEN.

1.4. Mission composition

Host organisation

Belgian Nuclear Research Center (SCK CEN)

Host facility

SCK CEN, SCH building

Mol, Belgium

Mission dates

1 February 2023 – 30 June 2023

2. Major Practices, techniques, methods, tools or systems operated or studied

2.1. Practice, technique, method, tool or system operated or studied during the mission

Deep learning meta-model for predicting effective tensor of hydraulic conductivity

Description

Our deep learning meta-model consists of a convolutional neural network followed by a feed-forward neural network (FNN). Convolutional neural networks (Goodfellow et al., 2016) (CNNs) are used to process data on regular grids, particularly images. In our case, the input spatial random field (SRF) of conductivity tensors is prescribed on unstructured meshes, and rasterisation is adopted to represent SRF on a regular grid. Datashader library (James A. Bednar & Wang, 2022) performs nearest-neighbour interpolation of an SRF into a 256x256 matrix of grey-scaled pixels. Since we consider tensors of conductivity on each element, three independent values of the 2D tensor are set for each pixel. CNN is used as a feature extractor from an input image. Appended FNN with three output neurons is employed for final regression. In the case of DFM models, random values prescribed on fractures can be stored in a separate channel or merged with values of bulk elements.

Usage

Deep learning meta-model is used to solve a regression problem using supervised learning. An unknown mapping of input random field to output effective tensors is learned from collected sample pairs of inputs and corresponding outputs of a model.

Benefits

Computationally cheap meta-model of numerical homogenisation can significantly reduce the computational cost of MLMC for DFM models. In tested cases, we achieved cost savings of around 50 %.

Limitations

Unstructured input data has to be rasterised for CNN. This procedure has to be included in the programming code. More importantly, necessary interpolation brings additional errors. However, for MLMC this error seems to be negligible.

Applicability

Deep learning meta-model plays an important role in the applicability of MLMC for DFM models. This faster alternative could significantly reduce the cost of modelling groundwater flow, contaminant transport etc.

2.2. Practice, technique, method, tool or system operated or studied during the mission

Spatially correlated random field (SRF) generation within MLMC homogenisation procedure

Description

Spatially correlated random fields of tensors of hydraulic conductivity represent input data for both DFM model and numerical homogenisation. Regarding numerical homogenisation within MLMC, a correlation length of a random field for a coarse sample on a finer level should be captured in a random field of a fine sample on a coarser level. In order to do that, we combine the GStools library (Muller & Schuler, 2021) (covariance model, SRF generation, …) and principal component analysis (PCA) to prescribe correlation length to tensor elements in an uncorrelated mode.

Usage

Samples from the standardised distribution of effective tensors are used to get PCA projection matrix. A correlation length is prescribed for covariance models of samples in PCA space. Samples are transformed back to the original space.

Benefits

For the sake of MLMC for a DFM model, this approach allows the creation of an SRF for samples on a coarser level from the effective tensors obtained by numerical homogenisation (or its meta-model approximation) on a finer level.

Limitations

Fitting a distribution of effective tensors might be time-consuming. Nevertheless, from the whole MLMC point of view, this cost is minor.

Applicability

This technique represents a suitable way to handle correlation lengths across levels of MLMC and can be used for various groundwater modelling tasks.

3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

This internship leads to the development of Python code that employs our existing MLMC Python package (Březina & Špetlík, 2022) for DFM models including numerical homogenization of the effective tensor of hydraulic conductivity and its faster meta-model based on deep learning techniques, in particular, convolutional neural networks combined with feed-forward neural networks.

Thanks to fruitful discussions with my mentor at SCK CEN, Eric Laloy, I was able to broaden my machine learning programming skills by combining the MLMC Python package with Python libraries and frameworks used for machine learning and AI, such as PyTorch or Optuna. PyTorch is used for meta-model design, training, and testing procedures. Optuna is adopted to find a suitable hyperparameter setting for the meta-model. It also gave me insight into different approaches to generating spatially correlated random fields than I had been using. Specifically, covariance models combined with principal component analysis give us a way to prescribe correlation lengths also for multidimensional distributions.

Based on the results achieved in the course of the internship, there is potential for two publications. To the best of my knowledge, MLMC for DFM models is itself an unpublished research area. In addition, the meta-model for numerical homogenization of the effective tensor of hydraulic conductivity is also poorly described in the literature. Not to mention, MLMC with a meta-model of numerical homogenization which is a completely new approach. The work done will form a significant part of my PhD thesis.

We will continue to build on the research carried out during the internship. Developed techniques will be used for other DFM problems to verify that the meta-model is beneficiary for a range of tasks. Our ultimate goal is to expand the approach to three dimensions, which amongst others will require changes in the rasterization procedure and in the structure of the metamodel itself.

3.2. Relevant findings and conclusions for home organisation

An essential outcome of the internship is a fast homogenization of the effective permeability tensor of a fractured porous media using neural networks. The fast homogenization enabled the application of the multilevel Monte Carlo method for the fractured media. This technique, if extended to 3d case, could improve accuracy or decrease the cost of the stochastic models used for the uncertainty analysis and performance assessment. Jan Březina, TUL supervisor, highly acknowledges the support from the EURAD project since these results would not be achieved without inspiration and collaboration with other teams in the DONUT work package. Personal thanks come to Eric Laloy, the supervisor on behalf of the hosting organization, for fruitful discussions and his essential expertise in the application of neural networks.

3.3. Relevant findings and conclusions for host organisation

Through this internship, the SCK CEN mentor, Eric Laloy, had the opportunity to learn the theoretical foundation and practical advantages and limitations of the popular MLMC framework to speed up MC calculations. Furthermore, mentoring this internship also allowed Eric Laloy to sharpen his knowledge of state-of-the-art deep learning techniques and their training, thanks to the amazing work performed by the trainee, [redacted].

APPENDICES

Mission journal

February 2023

- generating data for CNN training and testing procedures
- rasterising input 2D conductivity fields of conductivity tensors. Considering cases without/with fractures - rasterized images of shape 256x256x3
- developing Python code for dataset preprocessing, dataset loading, CNN model, CNN training and testing, data postprocessing and visualisation
- developing code for CNN training using optuna framework that can also run on cluster with portable batch system

March 2023

- Developing and refactoring code - more advanced CNN model class
- Hierarchical CNN (without fractures)
    - generating 3x3x3 data from already rasterized 256x256x3 data including recalculating of corresponding effective tensors
    - testing pretrained layers in hierarchy for larger images, up to 256x256x3
    - training whole hierarchy of CNNs at once

April 2023

- Standard CNN (without fractures)
    - finding suitable topology
    - testing regularisation techniques - dropout, batch normalisation, …
- Implementing more advanced way to generate input conductivity field: gstools library + principal component analysis
- Implementing vision transformer as alternative to CNN
- Adopting wide range of data preprocessing techniques (RobustScaler, QuantileTransformer, …)

May 2023

- CNN trained on data from DFM model with constant conductivity on fractures
    - conductivity on fractures merged into existing bulk channels in input data
    - conductivity on fractures included as separate (fourth) channel to input data
- CNN trained on data from DFM with non constant conductivity of fractures (conductivity calculated from aperture)

June 2023

- refactoring and accelerating rasterization procedure and homogenization samples generating code
- MLMC with homogenization
    - developing code that uses mlmc Python library
    - calculating homogenization samples and processing their results for coarser level
    - employing CNN meta-model instead of numerical homogenization

Mission bibliography

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Goodfellow, I., Bengio, Y., & Courville, A. (2016). *Deep Learning* (Illustrated edition). The MIT Press.

James A. Bednar, Jim Crist, Joseph Cottam, & Wang, P. (2022). *Datashader*. https://datashader.org/

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MISSION BENEFICIARY

[redacted]

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Eric Laloy (Engineered and Geosystems Analysis Unit, SCK CEN)

Home organisation experts

- Jan Březina (Institute of New Technologies and Applied Informatics, TUL)

REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
Date of last signee 23.7.2023	[redacted]	Jan Březina	Eric Laloy