MOBILITY MISSION REPORT

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REPORT TEMPLATE GUIDELINES — REMOVE THIS ENTIRE SECTION BEFORE SUBMITTING

- *This template consists of "sections" (fixed headings) and "fields" (text boxes for custom information)*
- *All sections and fields are mandatory unless specified otherwise*
- *Appendix "A. Mission journal" should be prepared during the course of the mission*
- *All template guidelines shall be replaced with custom text or removed as specified*
- *The report shall be approved by the official mission mentors or supervisors before submission (use the signature block at the very end of the report template)*
- *The report shall be submitted in both editable (.doc) and portable (.pdf) file formats*
- *Both files shall use the code of the mission as the filename's suffix, i.e. "Mission_Report_SXXXXX" : the word "Template" shall be replaced with the initial code assigned automatically to the application (letter "S" followed by 5 digits)*
- *The report shall be submitted via email to euradwp13@sckcen.be*

MISSION TITLE

DONUT - ACED workshop and visit at SCK CEN for work on metamodels for homogenization of processes in fractured media

DESCRIPTION

Concerned organisations

- Research entities
- Waste management organisations

My organization Technical University of Liberec, participates under Czech WMO : SÚRAO.

Concerned infrastructures or facilities

- High-performance computing

The mobility action was related to results using HPC.

Concerned phases

- Phase 2: Site characterisation
- Phase 5: Post-closure

Studied homogenization techniques are currently used in the description of the host rock properties (characterization), they are used within transport models for the post-closure phase.

Themes and topics

- Theme 4: Geoscience to understand rock properties, radionuclide transport and long-term geological evolution
  - Aqueous pathways and radionuclide migration
- Theme 5: Geological disposal facility design and the practicalities of construction, operations and closure
  - Facility and disposal system design
  - Constructability, demonstration and verification testing
  - Health and safety during transport, construction, operations and closure
  - Monitoring and retrievability
- Theme 7: Performance assessment, safety case development, and safety analyses
  - Performance assessment and system models
  - Treatment of uncertainties

Primary motivation of the collaboration is the development of fast homogenization methods enabling the use of the multilevel methods for speedup uncertainty propagation and variance-based sensitivity analysis involving the transport in fractured media.

Keywords

performance assessment; multilevel Monte Carlo method; transport in fractured media; numerical homogenization; neural networks

EXECUTIVE SUMMARY

First part of the mobility was a participation on the DONUT-ACED workshop, November 8 – 10, Belgium. Second part was a one week work visit at SCK CEN. The visit enabled better mutual understanding in usage of neural networks for numerical homogenization of fractured porous media. This topic is motivated by application of multilevel Monte Carlo method to transport in crystaline rocks.

1. MISSION BACKGROUND

1.1. R&D background

Multilevel Monte Carlo method could significantly improve the performance of some uncertainty quantification methods used within performance assessment. Unfortunately, the method is not directly applicable to the transport in crystalline rock. The method requires the construction of a hierarchy of approximation that is challenging do for the random discrete fracture networks.

1.2. Mission objectives

Participate in the ACED-DONUT workshop. A mutual better understanding of approaches to uncertainties in transport processes with Eric Laloy. Work on a paper about homogenizations using neural networks to facilitate multilevel approximations for MLMC.

1.3. Mission request

“The first part of the mobility will be active participation in the DONUT-ACED workshop, November 8 – 10, Belgium. The second part will be a one-week work visit at SCK CEN. The aim is to work on machine learning techniques for homogenization of fractured porous media in relation to the mobility and internship of my Ph.D. student Martin Špetlík.”

1.4. Mission composition

Host organisation

SCK CEN

Host facility

Mechelen conference center, SCK CEN office in Brussels, SCK CEN facility in Mol.

Mission dates

7 November – 17 November, 2024

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

Multilevel Monte Carlo method

Description

Hierarchy of approximations of a quantity of interest (QoI) is used to reduce the variance of a Monte Carlo estimate and significantly reduce computational cost.

Usage

The method provides computationally efficient statistical estimates for quantities with multi-fidelity approximations.

Benefits

Enable more exact uncertainty quantification models.

Limitations

Currently the method is not directly applicable to the models involving discrete fracture networks typical for crystalline rock.

Applicability

We are interested in application to the transport of radionuclides, with QoI related to the contaminant concentration on the surface or in other target domains.

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

Convolutional Neural Networks

Description

Machine learning technique used in image processing and computer vision. The same weight kernel is applied for every position in the image, vastly reducing the number of independent model parameters that have to be learned.

Usage

The homogenized fracture network and random field for the hydraulic conductivity are rasterized to a high resolution tensor field. The CNN approach is used to determine effective hydrulic conductivity tensor of the sample.

Benefits

CNN is computationally effective and known to deal well with similar scalar homogenization problems.

Limitations

The rasterization step must be done, increasing the computation time and contributing to numerical error.

Applicability

Resulting CNN-based model was successfully tested to speed up the homogenization necessary in the multilevel Monte Carlo for fracture media.

3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

Understanding of various machine learning techniques and their applications used by Eric Laloy and his colleagues from the host organization. Introduction to multiple-point statistics techniques and diffusion-based neural networks with applications in geoscience computations. Conclusion: steps toward common paper in homogenization, identification of possible areas of common interest for future collaboration.

3.2. Relevant findings and conclusions for home organisation

3.3. Relevant findings and conclusions for host organisation

3.4. Relevant findings and conclusions for other organisations

4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

4.1. Generic potentials

Great potential in neural networks in stochastic calculations, due to the speedup of models and efficient use of modern hardware. Potential for better interoperability of developed neural network models.

4.2. Potentials for home organisation

4.3. Potentials for host organisation

APPENDICES

Mission journal

7.11. travel

8.11. ACED-DONUT workshop

9.11. ACED-DONUT workshop

10.11. ACED-DONUT workshop,

11.11. Saturday, reading, preparation of topics for discussion

12.11. Sunday

13. 11. Detailed discussion about MLMC technique

14. 11. Detailed discussion about CNN, its implementation and training techniques.

15. 11. Research, scientific reading.

16. 11. Visit in Mol, underground laboratory

17. 11. Conclusions, future plans, travel back.

Mission bibliography

MISSION BENEFICIARY

Jan Březina
associate professor at Technical University of Liberec,
Czech Republic

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Eric Laloy

Home organisation experts

None

Other organisations experts

None

REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
9.2.2024	Jan Březina