Hessisches Kompetenzzentrum für Hochleistungsrechnen

Physics Meets Peace Research: Nuclear Verification with HPC

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Clusters
Lichtenberg II Cluster Darmstadt

Software
PyTorch

Additional Software
OpenMC, ONIX, Geant4

Institute
Science for Nuclear Diplomacy

University
Technische Universität Darmstadt

Introduction

In this peace research project, techniques for verifying the disarmament and arms control of nuclear weapons are developed. In addition, novel nuclear safeguards techniques are investigated, i.e., ensuring that nuclear material in civilian programs remains to be used for peaceful purposes only. While the initial motivation of the research originates in international security, verification and safeguards methods are of a technical nature and require the analysis of the underlying physical processes. In the nuclear field, this involves the simulation of numerous particles and their interactions with matter, rendering HPC systems an important asset for the development of these techniques. Our project is organized into two major sub-projects. Sub-project 1, Particle detection for verification, focuses on the interaction of particles with matter, which requires significant computational resources. The particles, emitted, for example, from nuclear reactors or weapons, or as a result of probing these objects with a separate particle source, have signatures that can be used to authenticate accountable items as warheads or to safeguard nuclear material. Sub-project 2, Nuclear archaeology and reactor simulations, focuses on the simulation of nuclear fuel cycles and reactors. Assessing a state's plutonium and highly enriched uranium (HEU) stockpiles allows us to directly infer the maximum number of nuclear weapons a state can produce from these two materials. To determine these inventories, the operation of the producing facilities can either be simulated directly, or inferred from forensic measurements taken at the facilities. Both approaches require extensive simulations, as well as the solution of an inverse problem in the latter case.

Methods

In sub-project 1, Monte Carlo simulations are being conducted using the Geant4 toolkit to analyze the interactions and signatures of particles. The feasibility of using Nuclear Resonance Fluorescence (NRF) as a non-destructive technique for the inspection of small modular reactors (SMRs), and the uniqueness of nuclear warhead signatures obtained with the neutron multiplicity counting technique, were studied. In sub-project 2, reactor simulations consisting of Monte Carlo neutron transport simulations alternating with material depletion calculations were conducted. In analyses where an inverse problem was to be solved, i.e., inferring the operation of the facility given particular forensic measurements of the facility, Gaussian Process Regression was used as a surrogate for the computationally expensive reactor simulations. The inverse problem was approached with Bayesian inference, where the posterior distribution, which describes the solution of the inverse problem, was calculated either with Markov Chain Monte Carlo (MCMC) approaches or normalizing flow-based invertible neural networks.

Results

In sub-project 1, models for new types of nuclear fuel have been created and their intrinsic radiation signatures simulated. In addition, models of plutonium pits and multiplicity counters have been created, with which multiplicity results have been simulated. In sub-project 2, multiple analyses have been conducted. One work focused on simulations of a civilian Chinese fast breeder reactor to estimate its potential plutonium production using publicly accessible input data. Another project simulated a fictitious, but realistic, nuclear fuel cycle to demonstrate the validity of the approaches and move beyond simplified proof-of-principle case studies. In another reactor simulation study, two different fuel charges of a US reactor were simulated and investigated to identify observables of major operational parameters, and in particular to differentiate between the charges. Two analyses focused on solving the above-mentioned inverse problem using deep-learning approaches and MCMC approaches, respectively, for the scenario of investigating high-level nuclear waste, a byproduct of reprocessing spent nuclear fuel.

Discussion

In sub-project 1, the intrinsic signatures serve as an important pre-requirement that will now be followed by implementing an NRF simulation workflow to probe fuel and SMR models. The multiplicity technique has been successfully simulated; more complex test item models will now be developed and studied with it. In sub-project 2, detailed information on the Chinese reactor's geometry and fuel composition is scarce, and therefore data from similar reactor types was used. This requires a broad discussion of the role of uncertainties and their impact on the estimation of plutonium production and will be conducted in future work. For the nuclear fuel cycle analysis, the results of the benchmark fuel cycle and the model agree well, and differences can be explained. The next step comprises solving an inverse problem and quantifying the accuracy. For the project with different fuel charges, the investigation of parameter reconstruction results and the subsequent refinement of the list of observables is ongoing. An investigation of a third fuel charge is envisioned. The analyses for the high-level nuclear waste were successful in reconstructing parameters with both computational approaches. Inverse problem scenarios in which the waste corresponds to one operational period, as well as mixtures of waste, i.e., mixed waste from different operational periods with multiple parameters to be reconstructed, have been solved. The mixture of waste scenarios are planned to be investigated further in the future.

Publications

Geiser R.; Mertes L.: "Breeding Uncertainties - A Simulation-Based Analysis of China’s CFR-600 Reactors and its Strategic Ramifications"; Science Peace Security; Aachen (Germany) 10-12 September (2025)

Merte L.; de Troullioud de Lanversin J.; Englert M.; Frieß F.; Göttsche M.: "Plutonium Production of the Chinese Fast Breeder Reactor"; AMC Conference; Uppsala (Sweden) 12-13 June (2025)

Unruh F.; Göttsche M.; "Applying neural networks in nuclear archaeology with nuclear reprocessing waste", DPG Conference; Bonn (Germany) 12-13 March (2025)

Pazos L.; Schnellbach Y.; Göttsche M.: "non-destructive Probing of Novel Reactors with Nuclear Resonance Fluorescence"; Science Peace Security; Aachen (Germany) 10-12 September (2025)

Pazos L.; Fichtlscherer C.; Kütt M.; Göttsche M.: "Uniqueness of Nuclear Warhead Neutron Signatures"; AMC Conference; Uppsala (Sweden) 12-13 June (2025)

Rademacher L.: "Differentiating between Plutonium and Tritium Production Modes using Nuclear Archaeology"; AMC Conference; Uppsala (Sweden) 12-13 June (2025)

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