The project addresses one of the key challenges in the development of nuclear energy based on fusion reactors. In such devices, structural materials are continuously bombarded by high-energy neutrons, leading to the formation of helium atoms within the metal. Helium does not dissolve in the crystal lattice; instead, it accumulates at structural defects and forms microscopic bubbles. Over time, these bubbles weaken the cohesion of the material, promote microcrack formation, and influence helium-induced embrittlement and the mechanical response of the material under different loading conditions, posing a serious threat to the reliability of fusion reactors.

To understand these processes, the project employs advanced atomistic modelling. Two new interatomic potentials will be developed, enabling computer simulations of millions of atoms. The first is an extension of an existing Angular-Dependent Potential (ADP) for iron–chromium alloys. The second, a machine-learned interatomic potential (MLIP), will provide near-DFT accuracy for complex defect structures. Both models will be constructed based on high-fidelity quantum-mechanical DFT calculations performed within the project and in collaboration with ICAMS (Ruhr-Universität Bochum) and MatéIS (INSA Lyon).

Once the potentials are developed, large-scale molecular-dynamics simulations will be performed. These will track helium atom migration in irradiated metals, their accumulation at defects, bubble formation, and their role in helium-induced embrittlement and the mechanical response of the material under different loads. The simulations will include helium interactions with radiation-induced defects formed by collision cascades, with grain boundaries, and with microcracks, reflecting the conditions materials experience in fusion reactors.

A key element of the project is experimental verification of the computational models. Steel samples will be irradiated using two complementary approaches:

• at the Nuclear Physics Institute of the Czech Academy of Sciences, via controlled implantation of helium ions followed by iron-ion irradiation to reproduce reactor-like conditions;
• at CERN, using high-energy proton pulses at the HiRadMat facility to generate highly localized and intense material damage.

The resulting microstructure, including helium bubbles, dislocations, and radiation-induced defects, will be analysed using TEM. Experimental data will serve to validate the computational models and assess their predictive capability.

The project will deliver the first comprehensive and experimentally validated models describing helium's influence on microstructure evolution and mechanical performance of steels used in nuclear-energy applications.