

## NOMATEN Online Seminar

**Time:** 1 PM

**Location:** gotomeeting room - <https://meet.goto.com/NCBJmeetings/nomaten-seminar>

**Seminar date:** February 6th, 2024

**Title:** How to model microstructure in FeCr under and out of irradiation: a phase field approach

**Speaker name:** Dr. David Simeone

**Speaker affiliation:** French Alternative Energies and Atomic Energy Commission (CEA), France

**Abstract:** Faced with major societal challenges (ecological crisis, energy crisis), it is essential to better understand the behaviour of materials in order to improve the lifespan of nuclear reactors as well as their safety. The properties of materials are dictated by their microstructure, so innovation requires knowledge of the microstructures of materials. With the increase in computing power, numerical simulation methods can be used to test theoretical models of microstructure formation under and outside irradiation. Among these methods, the phase field approach is proving very promising. It bypasses the limitations of atomistic methods (ab initio, molecular dynamics) and, thanks to its deep theoretical foundations, provides a useful guide for engineers. This presentation aims to present the fundamentals of phase field methods and their applications to simulate the complex nucleation process in the FeCr alloy under and without irradiation.

**Bio:** A 1993 graduate of CentralEsupelec, David Simeone began his career at the CEA's Nuclear Energy Division in Saclay (DES Division since 2020). A specialist in diffraction, he took an early interest in the development of condensed matter physics and numerical simulation techniques. In particular, he developed an original Rietveld grazing incidence analysis technique to characterize and quantify the evolution of the microstructure of materials irradiated by ions. At the same time, his research team has developed tools for modeling irradiation damage induced by ion, electron and neutron beams in materials (DART code). Finally, he is working on adapting phase field methods to model changes in the microstructure of materials subjected to external stresses (temperature fields, external stresses) and held out of equilibrium (irradiation effects). As a lecturer at Paris Saclay University, he is involved in national (Institut Intégratif des Matériaux) and international (delegate E-MRS) initiatives to promote innovation in materials.