The role of high performance computing in predictive models for microstructure evolution of irradiated Fe and FeCr alloys

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The quest to find the material with the best performance under irradiation, particularly for the extreme conditions expected in a fusion reactor, relies heavily on modeling and understanding the effects of radiation at a fundamental level. Methods to model microstructure evolution with informed parameters coming from *ab initio* calculations or molecular dynamics simulations are commonly used in this task. In recent years, these methods have become increasingly complex, due to the nature of irradiation and the fact that the system of interest for fusion applications are multicomponent such as FeCr or W alloys. High performance computing has become a necessary tool to apply these methods to increasingly more complex and realistic systems.

The development of these computational tools with predictive capabilities requires of experimental validation at different scales. With the advancement of experimental methods, with increased detail at the smallest scale, it is now possible to directly compare results of microstructure evolution to transmission electron microscopy (TEM) or atom probe tomography (APT), among other experimental methodologies. Much of this information comes from ion irradiation experiments and therefore must be carefully analysed if conclusions want to be extracted for neutron irradiation.

In this talk, an overview will be given on the simulation tools used to model microstructure evolution of irradiated metals, focusing on the case of Fe and Fe-based alloys. The multiscale modeling approach applied to this problem is described in detail as well as the need for HPC for such calculations. The connection of the simulation results and experimental observations will be given, discussing the limitations and needs for improvement.