Seminarske naloge:

- **Imperfections in crystalline metals and their influence on mechanical properties**
  - Introduction of 0D defects (vacancies, interstitials), 1D defects (dislocations), 2D defects (GBs), 3D defects (voids), describe how they emerge and evolve with strain, irradiation, ageing, how they affect the elasticity, plasticity (ductility, strength), few examples (like decrease of stiffness in porous media, GB strengthening, corrosion resistance).

- **FFT-based method for mechanical analysis**
  - The method should be introduced with corresponding equations and approximations, demonstrate applicability on a simple example, brief comparison to FEM.

- **Large uncertainties in fatigue life prediction**
  - One of the biggest unsolved issues in mechanical engineering is to understand why there is so large scatter in measured fatigue life of seemingly same specimens, what contributes to fatigue life (loading, material), how to model it, open issues.

- **Stress corrosion cracking (SCC)**
  - How is SCC different from general corrosion, where it applies in NPPs, what are the modelling approaches and issues (multi physics, multi scale), describe experimental facilities targeting SCC.

- **Quaternions as a useful tool to represent spatial orientations and rotations**
  - Introduction of quaternion number set, why it is useful, compare with other approaches for measuring crystallographic orientations and rotations (rotation matrix, Rodriguez vector...), introduce (inverse) pole figures and show few examples of usage.

- **Constitutive laws in crystal plasticity FE modelling**
  - Describe briefly crystal plasticity theory (slip systems in FCC, BCC, HCP lattices, and Schmid’s law), the role of constitutive laws (plastic flow, hardening) and their classification (phenomenological, physical-based), demonstrate the differences on few examples.

- **Homogenization methods used in crystal plasticity FE analysis**
  - What is a homogenization technique in FE analysis, why is it useful, demonstrate it on few simple examples.

- **Disruption forces in the divertor of DEMO tokamak**
  - Describe all types of forces (electrical, magnetic and mechanical) acting on the divertor cassette and pipes, estimate maximum amplitudes in normal DEMO conditions.
• **Thermo-current measurement diagnostic in the divertor of DEMO tokamak**
  o Introduce the thermo-current measurement diagnostic, why is it important, its challenges in DEMO environment, alternative approaches.

• **Non-destructive techniques for damage characterization of metallic pipes and vessels in NPPs**
  o Introduce the ultrasound (and other) technique using physical principles, show the limitations (what is the smallest detectable crack, how does detection of cracks depend on the distance from the sensor), few examples with simple crack geometry and size.

• **Ageing mechanisms in stainless steel components of NPPs**
  o Describe irradiation embrittlement, hardening and swelling, creep, thermal fatigue, SCC, IASCC, introduce basic principles behind each phenomenon and what are the engineering measures for its control, how we consider these mechanisms in simulations.

• **Method for the calculation of irradiation damage – in units of dpa – in metals**
  o Introduce the unit of dpa (displacement per atom) and the corresponding procedure(s) for its calculation in irradiated specimens (depending on the carrier of the radiation – proton vs. neutron, radiation flux and fluence), what are the associated uncertainties.

• **Approximate polycrystalline models and their range of validity**
  o Introduce Voigt and Reuss limiting models in the elastic regime of a polycrystalline, and Sachs and Taylor (Lin) limiting models in (elasto-)plastic regime, derive some tensile responses and compare them with FEM simulations on few simple examples.

• **Dislocation pile-up theory**
  o Phenomenological description of the pile-up mechanism of dislocations close to GBs, some analytical predictions of stresses along GBs.

• **Challenges in modelling crack initiation and propagation in polycrystalline metals**
  o Introduce the stress divergence (singularity) issue at a crack tip in elastic medium and the corresponding FE mesh convergence problem (describe situations when it is acceptable to have a singularity in the FE model), new field of fracture mechanics, alternative approaches (cohesive zone approach, xFEM).

• **Crystal plasticity theory**
  o Describe basic principles behind crystal plasticity, define slip systems for FCC, BCC and HCP lattices, Schmid’s rule, criteria for slip through slip flow equation and hardening equation (without size effects), kinematic relations in small and finite strain approximation, discuss the validity (applicability) of the theory in various metals.

• **Strain-gradient crystal plasticity theory**
  o In comparison to conventional crystal plasticity, describe basic principles behind strain-gradient crystal plasticity, difficulties in FE implementation.
• **Irradiation-assisted stress corrosion cracking (IASSC)**
  o Describe the IASCC phenomenon in austenitic stainless steel, was not anticipated in the design of internals in GEN2 NPPs (example of baffle bolt cracking), modelling approaches using CPFE method.

• **Hall-Petch or grain boundary strengthening in polycrystalline metals**
  o Introduce the influence of GBs as barriers to dislocation motion, hence the observed grain size dependence on measured flow stress in polycrystalline metals, try to rationalize the square-root dependence with grain size.

• **FE method in continuum mechanical analysis**
  o Basic equations and approximations behind FE analysis, show how a variational solution is achieved for the equilibrium of the forces and the compatibility of the displacements using the principle of virtual work for a volume that is discretized into finite elements, possibly mention xFEM for crack modelling.

• **Electron backscatter diffraction (EBSD) method**
  o Introduce the EBSD method using basic principles, describe what can be measured, precision, accuracy, colouring scheme, orientation triangle plots (pole and inverse pole figures).

• **Dislocation channelling in low stacking-fault-energy (SFE) steels**
  o Describe the mechanism of slip localization in the so-called thin channels (slip bands) that form in parallel within the (un-irradiated) grains, introduce SFE steels, their properties, what are the consequences of having slip channels, describe the modelling approaches.

• **Dislocation channelling in irradiated polycrystalline metals**
  o Describe the mechanism of slip localization in the so-called thin channels (clear bands) that form in parallel within the irradiated grains (highlight the difference from the un-irradiated case), their properties, what are the consequences of having slip channels, describe the modelling approaches.

• **Multi-scale approaches for modelling irradiation damage**
  o Introduce length and time scales associated with irradiation damage (cascade formation inside the crystal lattice as neutron collides with the atoms, resulting defects and consequent changes on mechanical properties after several years on macro scale), modelling techniques to effectively join the results on different scales.

• **What makes metals more or less prone to intergranular cracking?**
  o Focus on mechanical perspective (in contrast to chemical), introduce the concept of anisotropy and how it creates the grain mismatch effects resulting in higher intergranular stresses, also include the effects of loading geometry, grain topology, and texture.
• **Measuring elastic anisotropy of crystalline metals**
  o Relate the material elastic anisotropy with intergranular stresses, introduce several methods to calculate elastic anisotropy, discuss the possibility of extending the approach from elasticity to plasticity.

• **Interpreting Saint-Venant’s principle**
  o Introduce Saint-Venant’s principle, find various formulations of this principle in most structural mechanics textbooks and explore it particularly in the context of finite element analysis on a simple example.
Magistrske naloge:

- **Comparison between FE and FFT-based methods in polycrystalline tensile simulations**
  - The candidate should introduce basic equations relevant for FEM and FFT, discuss the similarities and differences between the methods, main advantages and main disadvantages, perform the FE simulations in Abaqus on simple PBC aggregate models to calculate macroscopic and local (intergranular) stresses, compare with available FFT simulations.

- **Estimation of disruption forces in the divertor of DEMO tokamak**
  - The candidate should build a FE model in Abaqus from a given divertor geometry, assign the proper electro-mechanical material properties and loading conditions relevant for DEMO tokamak environment, include Lorentz magnetic forces for constant (steady) currents and estimate the involved stress amplitudes within static approximation.

- **Are crack initiation sites correlated with high intergranular normal stresses emerging at these sites?**
  - The candidate should build a realistic 2D (later also 3D, if possible) FE model from the given experimental EBSD data of a polycrystalline stainless steel specimen free surface, assign the proper crystal plasticity model and simulate the tensile loading in Abaqus to compare the calculated intergranular stresses with micro-crack locations observed experimentally.

- **Algorithm(s) for efficient aggregate grain orientation assignment in FE models**
  - The candidate should find an efficient approach to assign the prescribed texture to a given aggregate FE model with given number of grains, in particular, to produce a desirable set of ratios of specific types of grain boundaries (like \(\Sigma_3\), \(\Sigma_5\), \(\Sigma_{10}\)) with the goal to investigate the possible positive influence of symmetric (\(\Sigma_3\)) grain boundaries on the intergranular normal stresses.

- **Identification of most influencing factors on intergranular normal stresses in a general polycrystalline metal**
  - The candidate should perform a sensitivity analysis with Abaqus solver of most important (mechanical) parameters that influence intergranular normal stresses (in statistical manner, by calculating the width of the distribution) in a general polycrystalline FE model, in particular, the influence of elastic material properties (elastic anisotropy), plastic material properties (Taylor factor, plastic strain), grain topology, (non-zero) texture, loading direction.

- **Approximate polycrystalline models used in mechanical analyses and their range of validity**
  - The candidate should introduce Voigt and Reuss limits of the elastic polycrystalline and Sachs and Taylor (Lin) limits of the elasto-plastic polycrystalline, highlight the approximations used in each of the limit, discuss the ranges of validity and derive the analytic solutions for stresses for particular loading conditions, and compare them with full-field FE simulations performed with Abaqus.
• **Influence of elastic anisotropy on intergranular normal stresses in FE aggregate model**
  - The candidate should find the relation between the elastic anisotropy (described by a single value through the universal elastic anisotropy index calculation) and intergranular normal stresses (described by the standard deviation) in the elastic regime of a random (zero textured) polycrystalline FE model assuming different loading directions (tensile, equi-biaxial), with possible extensions to finite textures.

• **Calibration of the crystal plasticity FE model for neutron-irradiated stainless steel**
  - The candidate should be able to perform FE simulations using the recently introduced micromechanical crystal plasticity model, developed by CEA, France and implemented in Abaqus solver, for neutron-irradiated stainless steel to fit the calculated tensile responses of an aggregate (representing the RVE limit) to available experimental data obtained from the literature at different irradiation levels.

• **Finding a structure’s best design with topology optimization**
  - The candidate should describe the basics of using the topology optimization method for a structural mechanics analysis, by introducing the penalization method, implement this method on a simple example (like a design of a bridge above the water given the mass constraint) by using the finite element analysis.

• **Finding a IGSCC resistant polycrystalline metal with texture optimization**
  - Given the elasto-plastic material properties of the grains, grain topology of the FE aggregate model and macroscopic loading conditions, the candidate should be able to introduce and apply the optimization method to identify an optimal set of crystallographic grain orientations (with, for example, zero overall texture) which would provide the smallest fraction of grain boundaries in an aggregate with very high intergranular normal stresses, therefore assuring the smallest susceptibility to IGSCC initiation.
Doktorske naloge:

- **Predicting intergranular crack initiation in a general polycrystalline metal model**
  - Intergranular (stress-corrosion) cracking (IGC or IGSCC) is a material degradation mode where crack initiation and crack growth correspond to the initiation and propagation of micro cracks at grain boundaries. Since local stresses at grain boundaries seem to be the driving force of IGC, they need to be accurately determined in order to quantitatively predict IGC initiation. From an engineering point of view, a reliable prediction of IGC initiation and especially dependence on the applied macroscopic loading is of the utmost importance as it can provide safe operating range of engineering components. A key goal of the proposed PhD thesis is to provide the physical understanding of IGC initiation behaviour by studying the intergranular stress distributions in a wide range of metallic materials based on the accurate calculation and understanding of the intergranular (normal and shear) stress distributions in metallic (uncracked) polycrystalline aggregate FE models under different loading conditions. In this way, the most influential (material, topological) parameters and related principles will be identified. We are looking for a candidate with BSc in physics or similar field with good programing skills; the candidate will be using commercial Abaqus FE solver, in-house Fortran and Python codes, and will have the opportunity to collaborate with the research group at CEA in France. Experience with FE modelling is beneficial but not required.

- **Numerical investigation of dislocation channelling in (un-)irradiated stainless steel**
  - In irradiated materials, the dislocation channelling refers to the localization of plastic deformation within slip bands (so-called clear channels) that appear to be free of radiation defects. A clear channel is a microstructural defect, only few tens of nm wide and with a length comparable with the grain size, which is created when loading an irradiated material. Its complex interaction with defects on the nanoscale affects the behaviour of the metal at the macroscopic scale (loss of ductility, reduced uniform elongation). In particular, because of their interaction with grain boundaries, with promotion of creation of cracks there, clear channels are also thought to have an important role in IASCC initiation. The current level of understanding is not sufficient to evaluate quantitatively their effect on IASCC and loss of ductility that are observed experimentally. In this respect, the PhD candidate will follow two approaches to investigate the effects of clear channels on the mechanical properties of metals. In the top-down (engineering-like) approach, the dislocation channelling should be imposed topologically to the aggregate FE with clear channels regions. Appropriate crystal plasticity laws should then be assigned to different model regions in order to reproduce the realistic responses of steel specimen on local and macroscopic scales. The effect of introduced dislocation channels on local stresses should then be investigated and a possible correlation with the initiation of intergranular cracking (IASCC) should be examined. In the bottom-up (physical-like) approach, the candidate will develop, implement and calibrate the strain-gradient crystal plasticity model to provide dislocation channelling in the aggregate FE model. Again, the influence of produced clear channels on intergranular stresses and IASCC initiation should be investigated. We
are looking for a candidate with BSc in physics or similar field with good programing skills; the candidate will be using commercial Abaqus FE solver, in-house Fortran and Python codes, and will have the opportunity to collaborate with the research group at CEA in France. Experience with FE modelling is beneficial but not required.