IRESNE 2024 INTERNSHIP SUBJECTS

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IRESNE
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cea iresne

Contents

About IRESNE

Research institute on nuclear systems for low-carbon energy production

IRESNE is the Institute for Research on nuclear systems for low-carbon energy production. Created on 1 February 2020 by the CEA, IRESNE brings together a team of 900 employees who design, simulate, test and qualify current and future nuclear reactors.

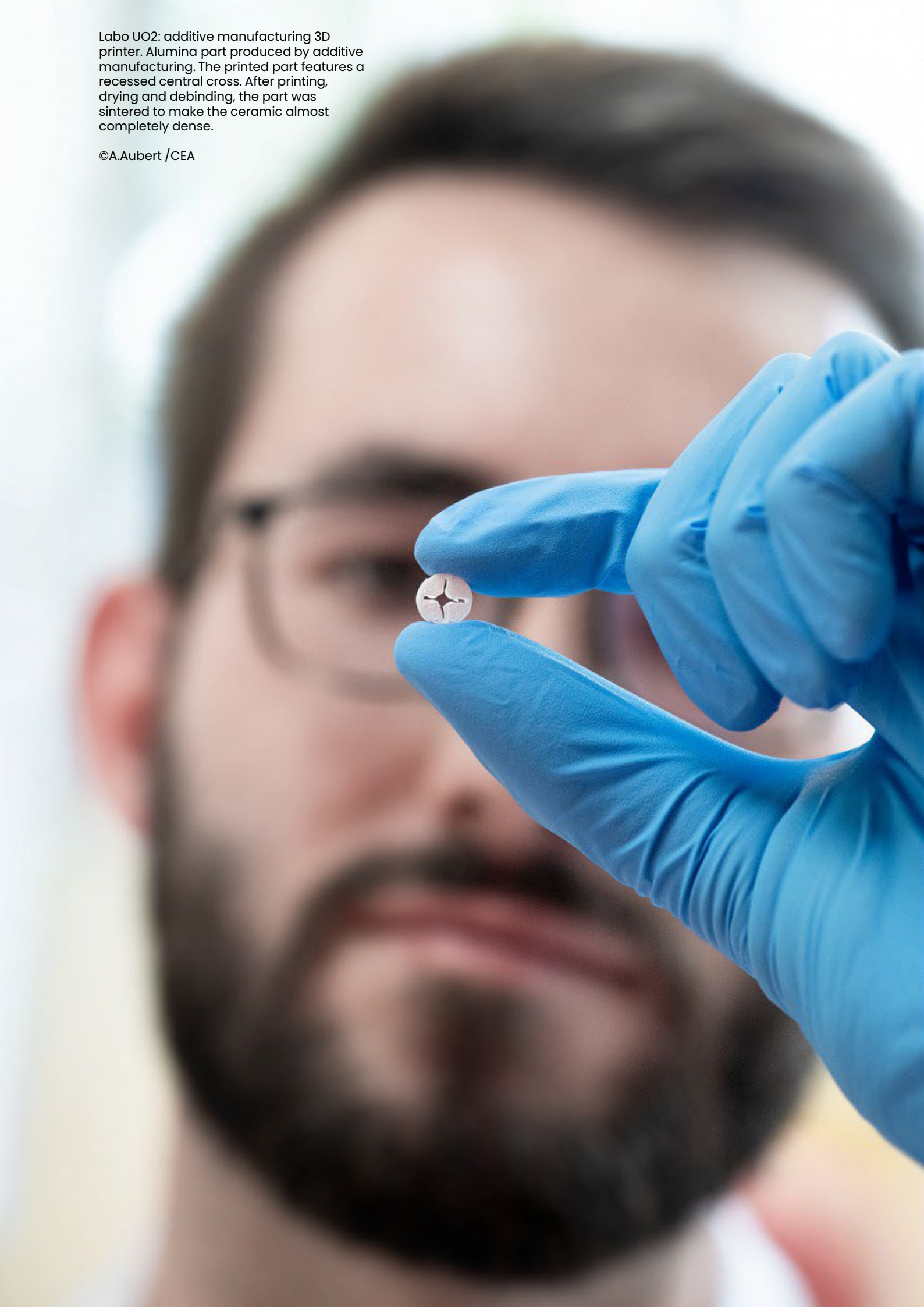
IRESNE is also opening up its field of research to the integration of nuclear systems into the low-carbon energy mix.
In addition to producing electricity, nuclear power is also a source of heat.

It is the technological innovations that support these two components - electricity and heat - that the institute focuses on in its research.

The aim of this optimization is to provide society with an energy mix that draws on all low-carbon resources.

The creation of the institute is part of the establishment, within CEA, of an organization dedicated to studies on decarbonized energies. This organization responds to the French government's desire to create a decarbonized energy mix based on nuclear power and renewable energies. The objectives are set by the French government within the framework of the Energy Transition Law for Green Growth and the Pluriannual Energy Programming (PPE) laws. These laws ensure the implementation of the National Low-Carbon Strategy (NLCS), France's roadmap for reducing greenhouse gas emissions. The NLCS concerns all sectors of activity and must be supported by everyone: citizens, local authorities and businesses.

To this end, the CEA has created an Energy Division (DES), which includes the IRESNE institute. The Department of Energies also includes an Institute of Applied Sciences and Simulation for Low-Carbon Energies (ISAS) and an Institute of Sciences and Technologies for a Circular Economy of Low-Carbon Energies (ISEC).



Labo UO2: additive manufacturing 3D printer. Alumina part produced by additive manufacturing. The printed part features a recessed central cross. After printing, drying and debinding, the part was sintered to make the ceramic almost completely dense.

IRESNE: A CEA institute at Cadarache

Located in the Provence Alpes Côte d'Azur region, in the commune of Saint-Paul lez Durance, the CEA-Cadarache center is at the heart of the energy transition with its research institutes and experimental platforms in the field of low-carbon energies: nuclear energy (fission, fusion), bioenergies and solar energies.

In addition to this research, Cadarache is also involved in nuclear propulsion for the French Navy, fundamental research in biosciences and biotechnologies, and studies on the decommissioning and dismantling of nuclear facilities and nuclear safety. Three institutes are actively involved in Cadarache research.

The mission of the CEA-IRESNE is to research and develop innovations in the field of nuclear fission energy (in particular reactors and nuclear fuels) as part of a low-carbon energy mix.

The institut for magnetic fusion research is working on fusion as a potential energy source for the future. Together with its international partners, the institute operates the WEST tokamak to prepare for future experiments on the international thermonuclear experimental reactor ITER.

The Aix-Marseille Institute of Biosciences and Biotechnologies (BIAM) explores two themes: the response mechanisms of living organisms (plants, algae, bacteria) to environmental constraints, and the bioconversion of energy to produce high-energy molecules.

CEA-Cadarache employs 2,400 people and is home to world-renowned research facilities, including the Jules Horowitz Reactor (RJH) currently under construction, the WEST/Tore-Supra tokamak, test bench for Iter, and the Cité des Energies.

The internships presented in this booklet are proposed by IRESNE, and all relate to the scientific and technological challenges facing the Institute. As indicated on some subjects, it may be possible to pursue a thesis at the end of the internship.

The international recognition of its researchers, the scientific quality of the studies carried out, combined with the uniqueness of the digital and experimental platforms of the Cadarache Research Center laboratories, offer future trainees a first-rate working environment for a successful internship. This will enable them to develop high-level skills that will be of great value to their career development.

Discover all CEA Cadarache internship offers on : https://www.emploi.cea.fr

POSEIDON platform: View of the test section (containing the fuel assembly mock-up) of the HERMES P loop.

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IRESNE internships in practice

Choosing to do an internship at IRESNE, at the Cadarache center, also means choosing a high quality of life.

The Cadarache Research Center, located in the commune of Saint-Paul-Lez-Durance (Bouches-du-Rhône), is ideally situated, 30 min from Aix-en-Provence, 1 h from the sea and 1 h 30 from the nearest ski resorts. It extends over a 900-hectare park planted with trees, where numerous animal species roam freely.

Trainees at Bac + 5 level receive a monthly internship allowance ranging from €700 to €1,300, depending on the school, degree and length of internship. A bonus may be awarded at the end of the internship, depending on the evaluation of the internship.

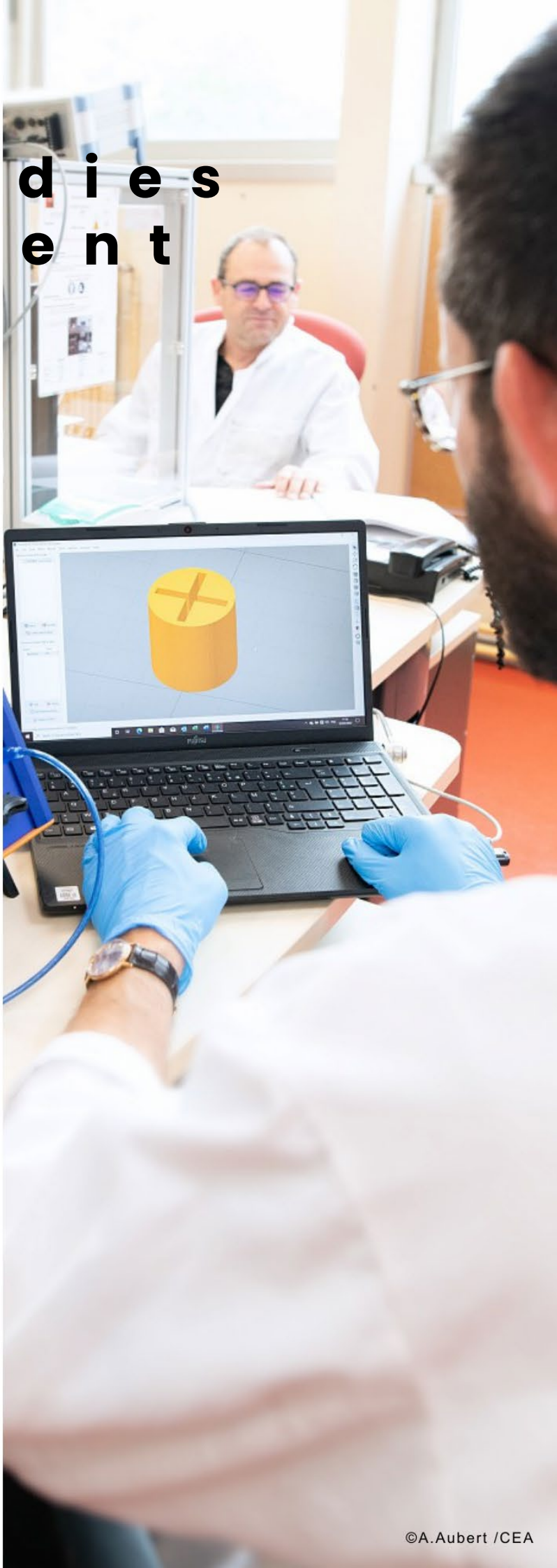
If the trainee rents accommodation for the duration of the course, the CEA may contribute to the accommodation costs. Trainees may also apply for housing benefit (APL).

A wide choice of accommodation in the 4 surrounding departments is available to trainees: for city dwellers, the towns of Aix en Provence (30 minutes by freeway), Pertuis (20 minutes by road), Manosque (10 minutes by freeway); for country lovers, the villages of Luberon, Var, Alpes de Haute Provence, ...

"Le Hameau" residence, just outside the Cadarache center, offers studio flats for rent. Address: Habitat Pluriel Résidence Le Hameau - 13115 Saint-Paul lez Durance, Telephone 04 42 57 43 83
The Cadarache Center is served morning and evening by buses departing from several towns and villages in départements 04, 13, 83 and 84. These buses are free of charge for people coming to work at the Center.

Two company restaurants are available at preferential rates for students.

Fuel Studies Department



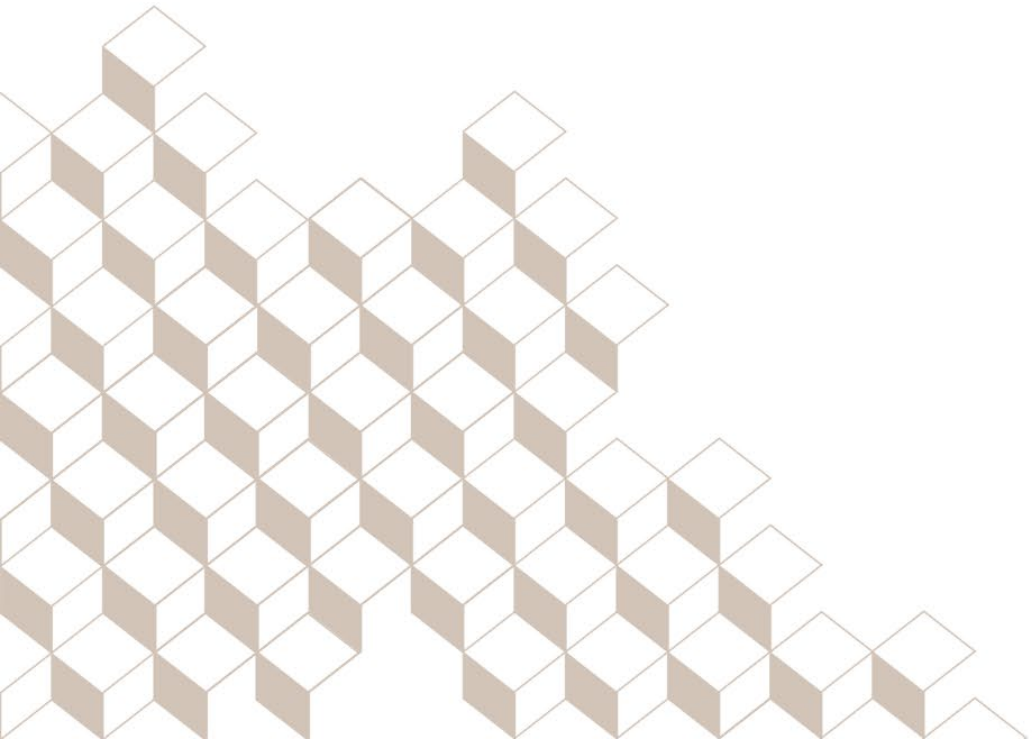
The Fuel Studies Department (DEC in french) focuses on nuclear fuel, with the aim of improving the performance and safety of current reactors (generations 2&3) and developing nuclear fuels for the reactors of the future (4th generation). Its mission is to acquire, integrate and capitalize on knowledge relating to the design, manufacture, characterization and study of the behavior of nuclear fuel elements in reactors. The DEC's activities combine numerical simulation/modeling and experimentation.

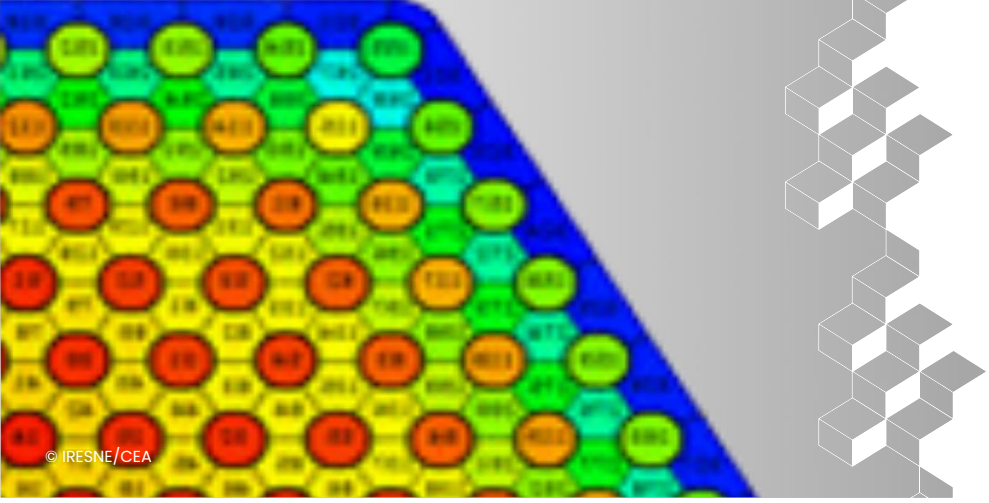
DEC is organized into three units:

- Analysis, Elaboration, Experimentation and Examination of Fuels Unit (SA3E).
- Studies and Simulation of Fuel Behavior Unit (SESC),
- Operating and Fuel Treatment Unit (SETC).

S E S C

Studies and Simulation of Fuel Behavior Unit





Assessment of SFR fuel pins thermalhydraulic and thermomecanical behaviours

DEC/SESC/LECIM & LEVA

In Fast Neutron Reactors (RNR or SFR), fuel elements, also known as pins, contain the fuel pellets which are inserted in a sealed metal cladding and are distributed in a triangular pitch in a hexagonal wrapper tube, the whole forming an assembly.

When the reactor is in operation, the power produced by the fuel is dissipated in the coolant. Depending on the location of the subassembly in the core, the coolant flow rate, or its proximity to control rods, the cladding maximum calculated temperature and its position in the assembly changes.

TRIO-MC, a scientific computing code, is specifically designed to assess the cladding temperatures and will allow, during this internship, to perform the thermohydraulic calculations of particular SFR assemblies, using a so-called "detailed" calculation scheme, required for such experimental subassemblies. The thermal behaviour of the clad will be validated from results of previous studies. Then, it will be possible to assess the fuel pin thermo-mechanical behaviour during irradiation from the fuel performance code GERMINAL and to compare the results obtained to available experimental data.

Objectives:
The objective of the internship will be, as a first step, to finalize the development of the pre/post treatment tool associated to TRIO-MC and GERMINAL OCS, specifically developed for experimental subas-semblies studied, and as a second step, to perform thermohydraulic and thermomechanical computations to assess the behaviour under irradiation of the fuel pins. Calculations will be performed for one or several experimental objects depending on the internship progress.

- Stage 1 : Familiarize yourself with TRIO-MC OCS and finalize the development of the pre/post treatment tool by automating some tasks,
- Stage 2 : Perform thermo-hydraulic calculations with TRIOMC, analyze and then validate the results from previous studies,
- Stage 3 : Perform thermo-mechanical calculations with GERMINAL, analyze and then validate the results from experimental available data.

Relations/collaboration:
Collaboration within the Fuel Studies Departement.

- **Desired schooling :**

Master 2 or final year of engineering school

- **Duration :**

6 months

- **Method/software(s):**

TRIO-MC and GERMINAL scientific computational codes under linux, python, MS Word Excel

- **Key words :**

SFR – thermohydraulic – thermomechanical behaviour – python

- **Thesis opportunity :**

No

- **Contact(s) :**

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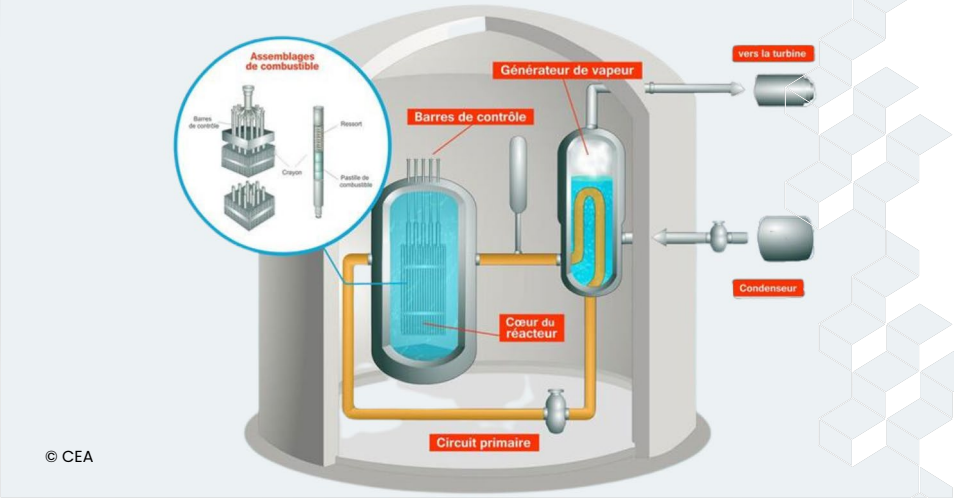

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Innovation in nuclear fuels: application of the C-K method to Accident Tolerant Fuels

DEC/SESC/LECIM & LEVA

The Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) is leveraging its experience in the field of nuclear fuels by applying its skills to a wide range of innovation projects.

These include the development of so-called "Accident-Tolerant Fuels" (ATF), whose objective is to improve the safety of Pressurized Water Reactors (PWRs) with respect to accidental scenarios such as Fukushima, while maintaining (or even improving) their performance in normal operation.

In this context, the LECIM is involved in a fuel innovation project, carried out in partner-ship with French industrialists, for which it is carrying out the design and thermomechanical dimensioning of ATF fuels. The aim of the internship is to revisit the field of ATFs through a mapping carried out using the C-K method, in order to identify innovation possibilities that may have been overlooked previously, as the studies carried out between 2014 and 2018 were essentially based on the adaptation of solutions already studied for other types of reactor.

The intern will therefore need to have a generalist profile, demonstrate curiosity, be comfortable exchanging with various experts in the field, be creative and have a good synthesis mind.

- **Desired schooling :**

Master 2

- **Duration :**

4-6 months

- **Method/software(s):**

C-K method (possibily ASIT method too)

- **Key words :**

Nuclear fuel, ATF, innovation

- **Thesis opportunity :**

Maybe : to be discussed

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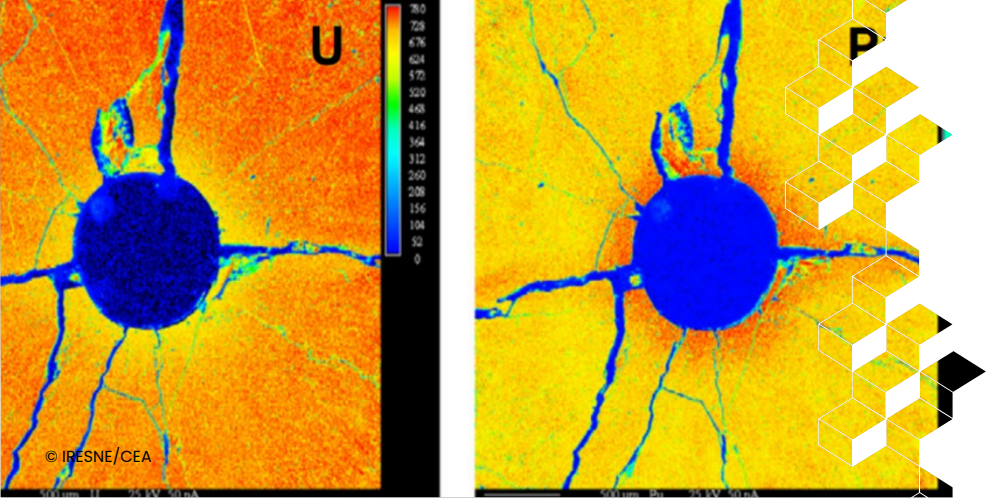

Multiphysics modeling of porosity transport under a temperature gradient

DEC/SESC/LEVA

In plutonium-uranium mixed oxides fuel (U, Pu)O2-x used in Sodium Fast Reactors (SFRs), the combination of high temperatures and steep temperature gradients causes the migration of fabrication porosities towards the center of the fuel pellets.

This phenomenon causes the formation of a central hole in the fuel pellets and a densification of the original microstructure, strongly affecting the thermal behavior of SFR fuel pins. In order to carry out studies and research, CEA develops computer codes that compute the thermomechanical behavior of nuclear fuels and works constantly to improve their models.

This internship focuses on improving the modelisation of the porosity transport, introducing a more thorough treatment of the thermodynamic representation of the fuel under irradiation and its inclusion in the multiphysics description of the phenomena. To this regard, the PLEIADES /GERMINAL has been coupled to the OpenCalphad thermodynamic code and to the Thermodynamics of Advanced Fuels - International Database (TAF-ID) database.

The goal of the proposed internship is to extend the multiphysics coupling between PLEIADES/GERMINAL and OpenCalphad to improve the modeling of (U, Pu) O2-x fuel restructuring. After a first familiarization with the modeling and theoretical approach, the candidate will integrate a new algorithm for the estimation of vapor pressures in the gas phase by OpenCalphad, compare the results obtained by the new approach to the legacy one, and perform a first validation of the coupled PLEIADES/GERMINAL/OpenCalphad/TAF-ID tool with analytical experiments

A successful internship could be followed by a Ph.D. thesis aimed at studying the mechanism of transport by evaporation /condensation by an advanced approach based on phase field modeling.

- **Desired schooling :**

Master of science – materials physics and chemistry

- **Duration :**

6 months

- **Method/software(s):**

C++, physico-chemistry of materials

- **Key words :**

Thermochemistry, nuclear fuel, Fast Breeder Reactors

- **Thesis opportunity :**

Yes

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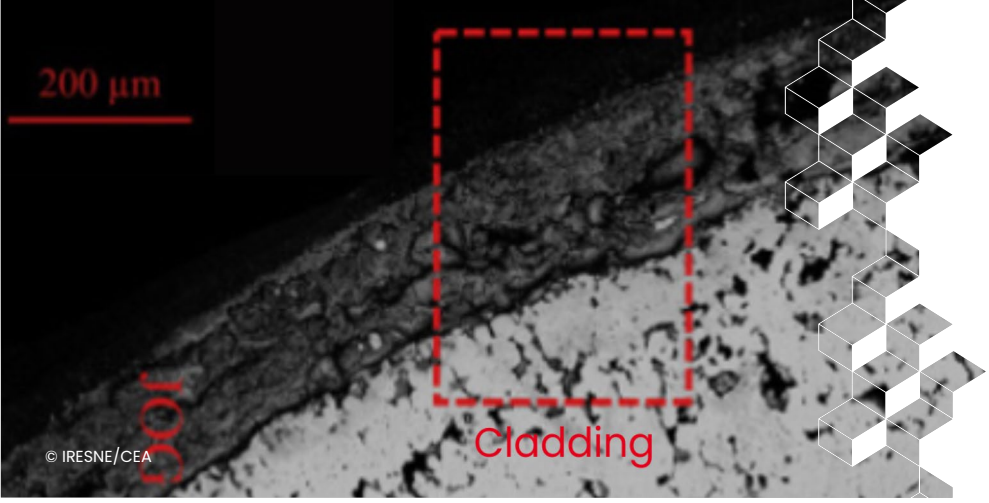

Thermodynamical calculations and modeling of cesium migration in fast reactor fuel pins

DEC/SESC/LEVA

Sodium cooled Fast Breeder Reactor (FBR) fuels are characterized by high operating temperatures and can reach high burn-ups at the end of their use. In these conditions, the fuel behavior is largely impacted by volatile fission products (cesium, etc.) released from the pellets and condensing under various chemical forms in the pellet-cladding gap.

These species modify the thermal exchange and in turn, all the other physical phenomena happening in the fuel pellet. In order to carry out studies and research, CEA develops computer codes that compute the thermomechanical behavior of nuclear fuels and works constantly to improve their models. This internship focuses on the modelling of long-distance migration of volatile fission products in the pin which can occur in FBR fuels during long irradiations.

A simplified model is currently under development to improve the computation of the fluxes and quantities of species in the pellet-cladding gap. An essential element of this model is an experimental law relating the quantity of mobile cesium and the temperature. In order to justify this law coming from international experience, the intern will :

- Carry out parametric thermodynamical calculations using CEA codes and the TAF-ID, a nuclear material thermo-dynamical database developed in an international framework (OECD/NEA), to understand empirical correlations and give them physical grounding,
- Improve understanding of the proportions of different phases in the gap (gaseous, liquid, solid) and their existence domain as a function of the quantity of species (uranium, plutonium, cesium, ...), temperature, or oxygen availability,
- Continue the development of the simplified model and its testing in fuel pin codes.

- **Desired schooling :**

Master of science – materials physics and chemistry

- **Duration :**

6 months

- **Method/software(s):**

Python, CEA scientific codes

- **Key words :**

Thermochemistry, nuclear fuel, Fast Breeder Reactors

- **Thesis opportunity :**

Yes

- **Contact(s) :**

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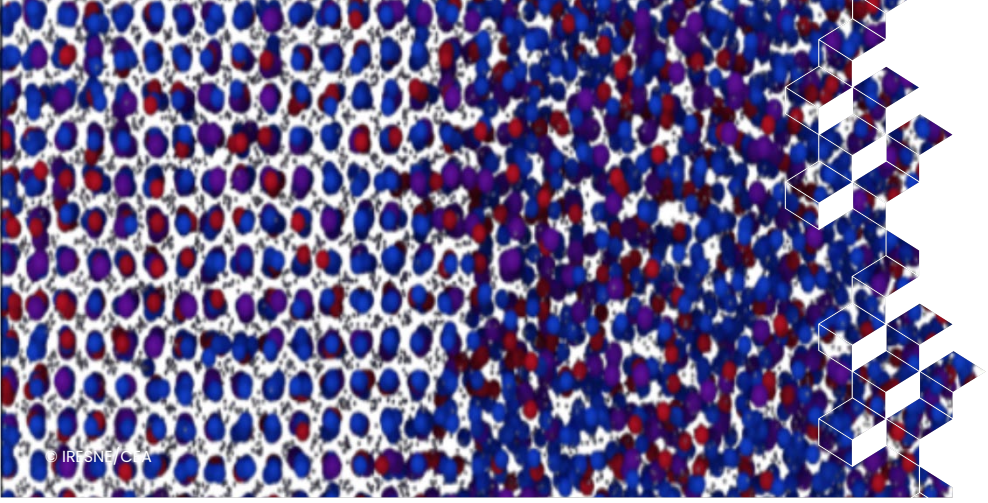

Calculation at the atomic scale of properties of plutonium and americium oxides

DEC/SESC/LM2C

The French nuclear strategy aims at multi-recycling the nuclear fuel (uranium dioxide, UO2) using the current pressurized reactors fleet or future fast neutron reactors. This will induce the use of plutonium-rich mixed oxide fuels incorporating small quantities of minor actinides, in particular americium or neptunium.

These changes in the fuel composition may cause important modifications of its in-pile behaviour and impact safety. It is thus crucial to know precisely the properties — in particular structural and thermal — of these compounds, such as the thermal expansion, the specific heat capacity or the melting temperature, as a function of their composition (various actinide and oxygen contents).

Atomic scale modelling is now an essential complement to experiments allowing one to determine numerous structural, thermodynamic, mechanical and electronic properties to predict in-pile behaviour of materials. Our laboratory combines electronic structure calculations with empirical interatomic potentials to determine systematically the properties of interest of nuclear fuel compounds as a function of composition and temperature.

This internship is part of a larger work aiming at improving the knowledge of the U-Pu-Am-Np-O system and will focus on the study of the Pu-Am-O subsystem using an empirical interatomic potential which will be developed by the intern. Electronic structure calculations will also need to be performed to provide data for the potential optimization.

The beginning of the internship will be dedicated to a literature review on the methods used and the materials studied. Electronic structure calculations will be performed and their results will be used for the optimization of an empirical interatomic potential. This potential will then allow for the systematic determination of properties of $(Pu,Am)O_{2-x}$ compounds. The results obtained will be used in the CEA thermodynamic databases and fuel performance codes used for the modelling of the fuel element.

- **Desired schooling :**

Engineering school, Master's degree, Solid state physics, Computational physics/chemistry

- **Duration :**

5 to 6 months

- **Method/software(s):**

UNIX / Linux
LAMMPS and VASP codes

- **Key words :**

Nuclear fuel
Atomic scale modelling
Fundamental properties

- **Thesis opportunity :**

Yes

- **Contact(s) :**

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Thermomechanical finite element design of reactivity control systems

DEC/SESC/LECIM

As part of the next generation of nuclear reactors, CEA and its partners are in charge of designing a fast neutron molten salt reactor, the main objective of which is the transmutation of minor actinides, in particular americium.

To date, France's approach to the management of radioactive materials and waste is based on deep geological disposal and on transmutation of minor actinides. Americium has been identified as the first target of a possible separation-transmutation strategy, the aim of which would be to reduce the long-term harmfulness of final waste. In this context, the ISAC (Innovative System for Actinides Conversion) project, which brings together all the French nuclear industry (CEA, CNRS, EDF, FRAMATOME, ORANO), has set out to respond to expectations regarding the management of long-lived nuclear waste by proposing a breakthrough alternative based on transmutation in a molten salt reactor (MSR). The aim of ISAC is to study the feasibility of the MSR "actinide converter" by carrying out a sketch study (evaluation of design options, concept performance, operating and safety analysis). The object selected is a fast-spectrum chloride salt MSR with inventory and supply of minor actinides, and is called ARAMIS-A for "Advanced Reactor for Actinides Management In Salt with Americium".

As part of the ISAC project, LECIM is responsible for the design and pre-dimensioning of reactivity control systems. An initial design phase, combined with analytical pre-dimensioning of these systems, has already been carried out. The main objective of the internship is to continue the design and dimensioning work on these systems by setting up finite element simulations. To this end, the LICOS tool of the PLEIADES platform will be used, and thermomechanical dimensioning will be carried out using the RAMSES II methodology (Rules for the Mechanical Analysis of Irradiated Structures).

The different steps of the internship could be as follows :

- Familiarization with the LICOS tool and modeling of ARAMIS-A reactivity control systems.
- LICOS calculations and sensitivity studies on design parameters.
- Depending on the results obtained, some design optimizations may be proposed.

- **Desired schooling :**

MASTER 2 with competencies in thermomechanical simulation.

- **Duration :**

6 months

- **Method/software(s):**

Finite elements computations with LICOS code.

- **Key words :**

Design, MSR, finite elements, reactivity control.

- **Thesis opportunity :**

No

- **Contact(s) :**

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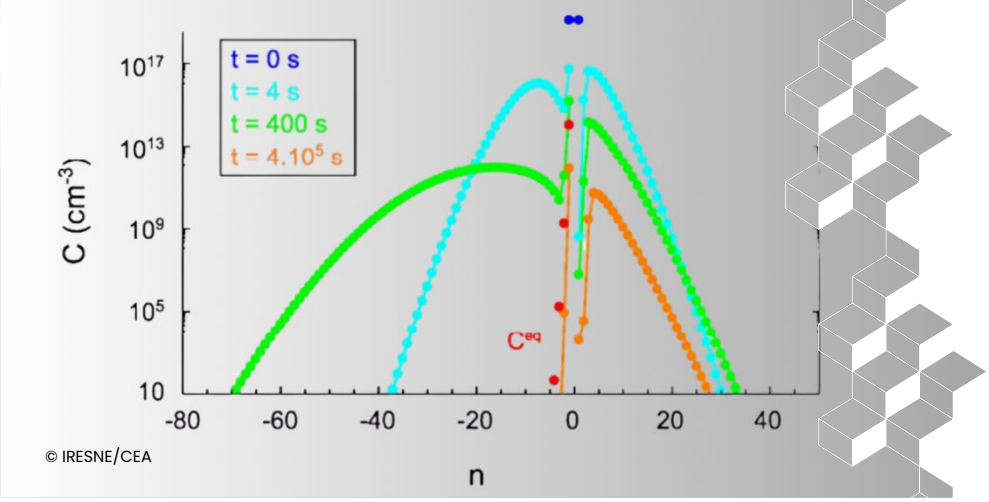

A hybrid atomistic-empirical numerical twin to predict the microstructural evolution of fuel under irradiation

DEC/SESC/LM2C

Like other industrial sectors, the nuclear industry is developing 'digital twins', applications that simulate the behaviour of an industrial component, such as a car, plant, reactor or, in our case, a fuel rod. The proposed work is part of this approach and contributes to the development of a digital twin of a grain that can be used to simulate its microstructural evolution under irradiation.

The microstructure of nuclear fuel (uranium oxide) is severely damaged during irradiation in a reactor: the atoms produced by the fission of uranium nuclei displace the atoms in the material in a cascade, creating irradiation defects (vacancies and interstitials) whose aggregation leads to the gradual appearance of cavities and dislocation loops. These extended defects influence the volume of the material, its creep and its retention of fission gases. The physical model of the phenomenon is cluster dynamics: a set of kinetic equations representing the chemical reactions of defect aggregation by diffusion in the material.

Most of the model parameters are derived from atomistic calculations (defect formation and migration energies, irradiation damage). However, some of them have not been calculated and are practically impossible to measure directly. The approach proposed for this internship is twofold:

1. Fitting the missing parameters using the model to simulate the results of experiments (already available in the laboratory) in which the microstructure is affected, such as transmission electron microscopy characterisation of dislocations and voids (size, concentration). Innovative techniques will be used:
   - Sensitivity analysis to determine which parameters affect the measured values
   - Optimisation (genetic algorithms) to fine-tune these parameters. The URANIE™ platform developed by the CEA will be used for the statistical analysis of the data.
   - Kinetic Monte Carlo for the damage simulation.
2. Validate this fitted model by comparing its results with measurements from other experiments. The model will then be applied to new situations, such as irradiation of fuel material to predict fission gas release, or the density of loops and dislocation lines.

This modelling project involves a variety of tasks:

- Interpretation of experiments
- simple computational development of optimisation scripts for URANIE
- simulation of experimental or industrial situations

This internship offers the candidate the opportunity to contribute to the development of numerical physics applied to multiscale modelling, taking a central position and a synthetic point of view. It is also an opportunity to discover for oneself how microscopic computational approaches ultimately help to solve complex practical problems.

R. Skorek, Étude Par Dynamique d'Amas de l'influence Des Défauts d'irradiation Sur La Migration Des Gaz de Fission Dans Le Dioxyde d'uranium, PhD Thesis, Univ. Aix-Marseille, 2013.
E. Gilabert, D. Horlait, M.-F. Barthe, P. Desgardin, M.-L. Amany, G. Carlot, M. Gérardin, S. Maillard, and T. Wiss, D2.2 - Behaviour of Fission Gases and Helium in Uranium Dioxide, EC report, 2020.

- **Desired schooling :**

Master's degree or equivalent in materials physics, modelling or numerical physics

- **Duration :**

6 months

- **Method/software(s):**

Using/improving simulation codes, simple coding of physical mechanisms

- **Key words :**

Numerical Physics
Chemical Kinetics
Materials irradiation

- **Thesis opportunity :**

No

- **Contact(s) :**

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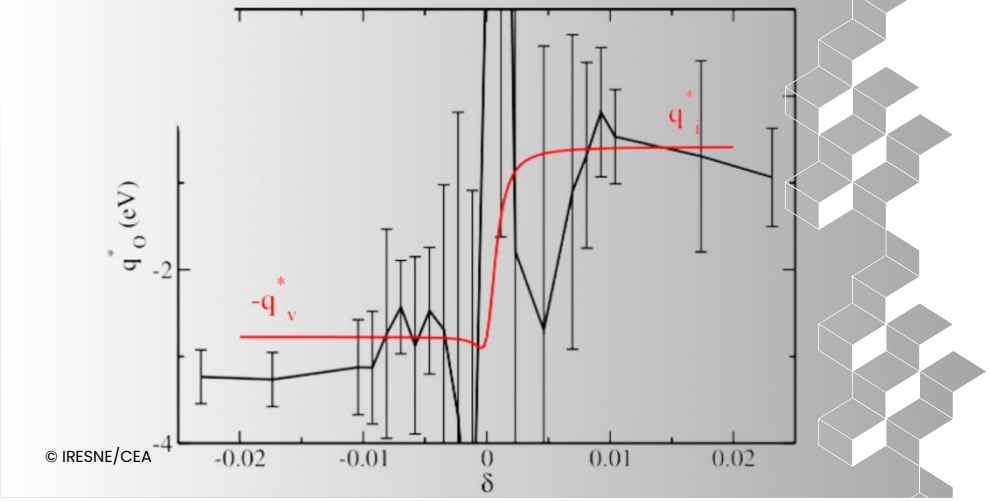

Molecular dynamics simulation of thermodiffusion in nuclear fuel materials

DEC/SESC/LM2C

Materials science is increasingly relying on multiscale simulation to address the complex in-reactor behaviour of nuclear materials, be it at the scale of the component (continuum mechanics,...), of the grain (phase field, rate theory...) or of the atoms (atomistic simulations). Thermodiffusion in nuclear fuel (UO_2) is a phenomenon whose complexity requires such an approach [1].

During irradiation, the fuel may experience a high thermal gradient that triggers the oxygen atoms migration (thermodiffusion). This phenomenon, inducing changes in the chemical characteristics of the material, is poorly understood at the microscopic level. Its key property, the heat of transport Q*, is an input parameter for the thermodiffusion model of the PLEIADES platform [2]. Unfortunately, it is very difficult to measure and, moreover, strongly affected by the physicochemical in-reactor evolution of the material.

Many atomistic simulations of thermodiffusion have been performed at the laboratory. Several methods for Q* evaluation have been tested; they provide very different results. The internship is aimed at understanding the cause of these discrepancies: simulations on simpler materials and situations will be carried out in the view of a better understanding of the mechanisms and of an improvement of the methods for Q* calculation.

The candidate will have the opportunity to develop skills in Statistical Physics, at and out of equilibrium, as well as in atomistic calculations with standard polyvalent molecular dynamics codes (i.e. LAMMPS) in which the laboratory is expert. Furthermore, these skills can be applied to a large spectrum of materials in various industrial fields such as electrolytic or thermoelectric materials (electronic industry) or liquid mixtures (petrol industry).

This project is connected to the development of the fuel simulation platform (PLEIADES) gathering in a single environment the models corresponding to all the phenomena involved in the material evolution (mechanics, physico-chemistry, thermodynamics, neutronics). In this context, the laboratory contributes to the computation of material properties used as input parameters for the platform, based on a multiscale approach coordinating atomistic calculations up to larger scale simulations. This working environment comprising physicists, computer scientists and digital experts all together is a key opportunity to discover a large panel of professions in numerical physics and computer science. This internship offers the opportunity to discover by oneself the way microscopic computational approaches finally helps solving complex practical issues.

[1] Schelling et al., Journal of Applied Physics, 112:8, 2012.

[2] Konarski et al. Journal of Nuclear Materials 519:104, 2019

- **Desired schooling :**

Master's degree or equivalent in solid state physics, modelling or numerical physics

- **Duration :**

6 months

- **Method/software(s):**

Molecular Dynamics code LAMMPS

- **Key words :**

Numerical, Statistical Physics, Molecular Dynamics

- **Thesis opportunity :**

No

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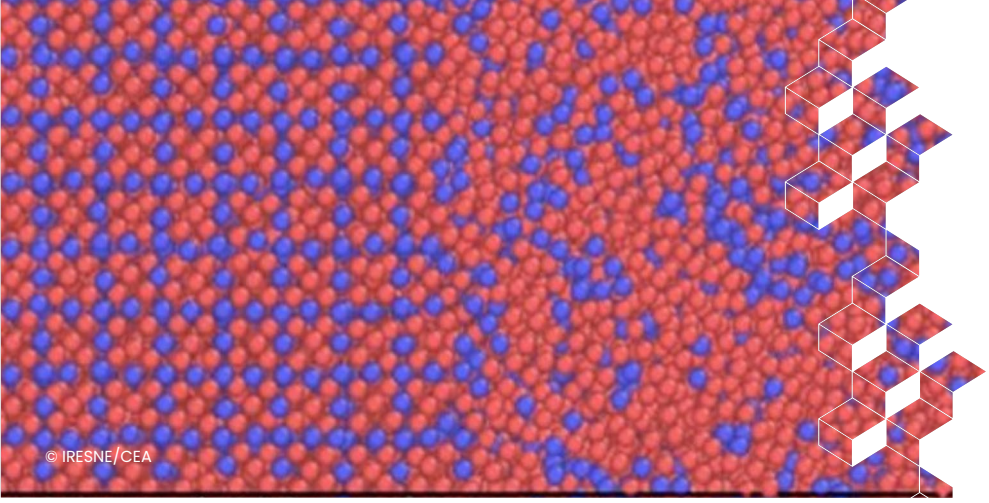

Investigation of nuclear fuel melting with deep-learning image analysis

DEC/SESC/LM2C

Artificial intelligence (AI) plays nowadays a crucial role in the design and innovation of materials for energy production and storage. The goal of this internship is to use AI-based image analysis methods to determine the melting temperature of nuclear fuels, a critical parameter to ensure reactor performance and safety.

The transition to low-carbon electricity production requires the design of innovative materials for energy production and storage. Research in this field relies more and more on numerical simulations aided by artificial intelligence (AI). In nuclear reactors, simulating fuel behavior under normal and accidental conditions improves reactor efficiency and safety. However, the complex phenomena triggered by irradiation within the fuel crystal structure lead to a highly complex evolution of macroscopic properties, which makes their simulation challenging. Thanks to AI, fuel behavior models can be improved, enabling the simulation of more complex systems, and accelerating the design of materials with optimized properties. In addition, deep-learning image analysis can be employed to analyze experimental and simulated microstructures, and extract crucial information for the understanding of the physical phenomena at play.

The objective of this project is to apply recently developed AI methods to study the melting properties of nuclear fuels. The melting temperature is a critical parameter that is challenging to determine experimentally due to the difficult handling of radioactive materials and the high temperatures involved. Through molecular dynamics simulations, it is possible to model the melting of the crystal lattice. However, the loss of regularity in the atomic structure occurs very gradually with increasing temperature, and conventional structural analysis methods cannot accurately determine the transition point between the solid and liquid state.

The candidate will use newly developed techniques to encode crystal structures into images, and then use them to train neural networks aimed at the classification of the simulated crystal structures. This will enable the determination of the melting temperature and the formation energy of various types of fuels, such as actinide oxydes and molten salts.

- **Desired schooling :**

Applied mathematics
Computational physics
Solid state physics
Materials science

- **Duration :**

6 months

- **Method/software(s):**

Molecular dynamics
Python, TensorFlow

- **Key words :**

Artificial Intelligence
Nuclear Fuels
Computational Materials

- **Thesis opportunity :**

Yes

- **Contact(s) :**

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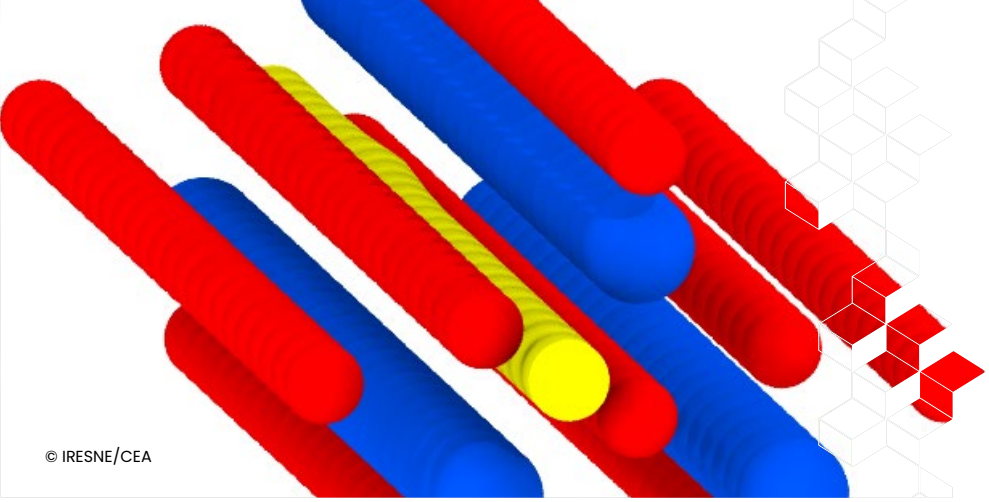

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Molecular dynamics study of dislocation mobility and annihilation in nuclear fuel

DEC/SESC/LM2C

Uranium dioxide UO_2 and mixed oxide $(U,Pu)O_2$ are the reference nuclear fuels in PWRs. Understanding the mechanical behavior of these polycrystalline nuclear fuels coupled with irradiation effects is a significant safety concern in nuclear engineering.

In this context, being able to assess the stresses and deformations occurring within the grains of the polycrystal and at their interfaces is an important objective. This involves understanding the phenomena at play at the scale of the microstructural heterogeneities of the fuel.

Objectives:
The main objective of this internship is to study the mobility of dislocations, which are the drivers of mechanical behavior in nuclear fuels UO2 and (U,Pu)O2, through atomic-scale simulations. These small-scale calculations will feed into a plasticity model for simulating compression experiments using the finite element method.

Building upon a methodology developed in the laboratory, the first step of this project will involve determining the velocity laws of edge dislocations in (U,Pu)O2 as a function of temperature and applied stress. The results will be compared to those existing for UO2 fuel.

The second objective will be dedicated to evaluating a parameter that reflects the critical spacing between screw dislocations beyond which their interaction leads to their annihilation, a phenomenon known as restoration. Once the parameter is determined, it will need to be tested in a mechanics model developed in the laboratory to compare simulation results to existing experimental data in the literature.

Stages of the internship:
The intern will begin the internship with a literature review phase to gain a comprehensive understanding of both the context surrounding nuclear fuel and the underlying physics related to the topic of the internship, including solid-state physics, crystal plasticity, and dislocation dynamics. Concurrently with the literature review, there will be a hands-on phase to become familiar with computational tools (Linux environment, TGCC supercomputers, LAMMPS code, OVITO post-processing software). Finally, the intern will transition into a phase of production and analysis of simulation results.

Work environment:
The intern will be welcomed within the Fuel Behavior Modeling Laboratory located at the Cadarache site. This highly dynamic laboratory specializes in modeling the fundamental properties and behavior of nuclear fuels and consists of 11 permanent researchers and an equal number of doctoral students.

- **Desired schooling :**

Master 2

- **Duration :**

5 to 6 months

- **Method/software(s):**

Molecular dynamics / LAMMPS / OVITO / Linux environment

- **Key words :**

Nuclear fuel, cristal plasticity, dislocations, molecular dynamics

- **Thesis opportunity :**

Yes

- **Contact(s) :**

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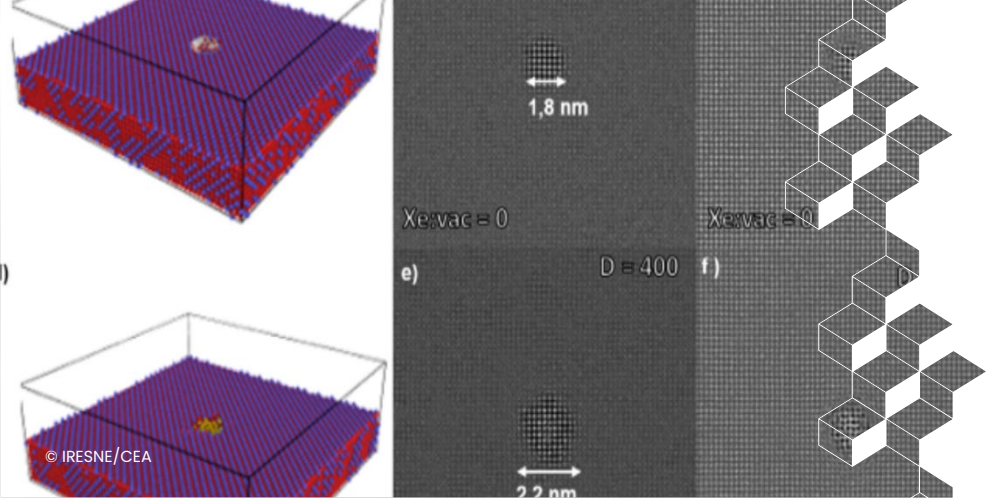

Improvement of a « machine-learning » interatomic potential for the simulation of nuclear fuels in classical molecular dynamics

DEC/SESC/LM2C

Irradiation phenomena in reactors lead to the presence of defects within the UO2 poly-crystals. This includes uranium or oxygen atoms in interstitial positions, or fission products (FPs) including gaseous FPs such as Xenon and Krypton. The presence and accumulation of those defects has an impact on the thermophysical properties of the fuel and an influence on nuclear safety scenarios.

The improvement of our understanding and modelling of the stability and agglomeration processes associated to those defects is therefore of fundamental importance. Experimental measurements performed with Transmission Electron Microscopy allow for the generation of detailed maps of nanometric defects within irradiated fuels. However, a calibration investigation would improve the accuracy of those measurements. We propose to perform this calibration leveraging atomistic simulations.

Objectives:
The objective of this internship is to contribute to the improvement of the interatomic potentials developed at the laboratory. Within an ongoing Ph.D. study, a machine-learning interatomic potential has been developed for UO_2 from first-principles calculations. The intern will add to the model the interactions between Xenon, Uranium and Oxygen atoms. Then, this new model will be used to perform molecular dynamics simulations of Xenon agglomerates (such as bubbles) within UO_2. A comparison between those simulation results and the TEM images will be performed and analyzed.

Steps:
Bibliography, familiarization with the computational tools (Linux environment, LAMMPS and ABINIT codes for the atomistic simulations, CEA super-computers), understanding of the machine-learning inter-atomic potential for UO_2 as well as its application for classical molecular dynamics calculations, comparison between the obtained simulation results and the existing TEM images.

Context and collaborations:
The internship is hosted in a very dynamic research laboratory specialized in the multiscale simulation of nuclear fuels, on the Cadarache research center. The intern will work in close collaboration with PhD. students at the laboratory, as well as with researchers from other CEA services.

- **Desired schooling :**

Masters degree in solid state physics or equivalent.

- **Duration :**

6 months

- **Method/software(s):**

LAMMPS, ABINIT

- **Key words :**

Solid state physics, Materials Science.

- **Thesis opportunity :**

Yes

- **Contact(s) :**

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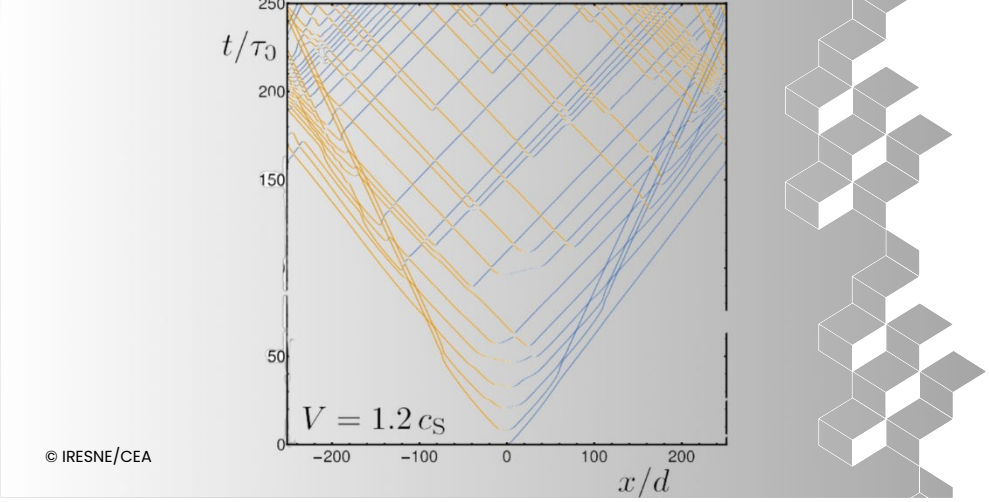

HPC Parallel Integrodifferential Solver for Dislocation Dynamics

DEC/SESC/LMCP

Understanding the behavior of metals at high deformation rate [4] (between 104 and 108 s-1) is a huge scientific and technologic challenge. Their irreversible (plastic) deformation is caused by linear defects in the crystal lattice : these are called dislocations, which interact via a long-range elastic field and contacts.

Nowadays, the behavior of metals at high deformation rate can only be studied experimentally by laser shocks. Thus, simulation is of paramount importance. Two approaches can be used at the mesoscopic scale of dislocations ensembles : molecular dynamics and elastodynamics simulations.

This PhD thesis follows the second approach, based on our recent works [1, 2], thanks to which the first complete numerical simulations of the Dynamic Peierls-Nabarro Equation (DPN) [5] was performed. The latter equation describes dynamic plasticity, accounting for retardation in elastodynamic interations between dislocations. (See also [3] for the same mathematical phenomena in the context of fractures.)

The DPN is a nonlinear integrodifferential equation, with two main difficulties : the non-locality in time and space of the involved operators. We simulated it thanks to an efficient numerical strategy [1] based on [6]. Nevertheless, the current implementation is limited to one CPU –thus forbidding thorough investigations on large-scale systems and on long-term behaviors.

Objective :
Based on the algorithmic method of [1], implement a HPC solver (High Performance Computing) for the PND equation, parallel in time and space, with distributed memory. This will be a preliminary step for the upcoming PhD.

Candidate profile :
The candidate shall have a solid background in scientific computing applied to Partial Differential Equations. Mastering C++ with OpenMP and MPI is recommended. Moreover, interest and knowledge in physics or continuum mechanics will be a plus.

[1] Pellegrini, Josien, Shock-driven motion and self-organization of dislocations in the dynamical Peierls model, submitted.
[2] Josien, Etude mathématique et numérique de quelques modèles multi-échelles issus de la mécanique des matériaux. PhD Thesis. (2018).
[3] Geubelle, Rice. J. of the Mech. and Phys. of Sol., 43(11), 1791-1824. (1995).
[4] Remington et coll., Metall. Mat. Trans. A 35, 2587 (2004).
[5] Pellegrini, Phys. Rev. B, 81, 2, 024101, (2010).
[6] Lubich & Schädle. SIAM J. on Sci. Comp. 24(1), 161-182. (2002).

- **Desired schooling :**

M2 in scientific computing/Numerical analysis, Physics

- **Duration :**

6 months

- **Method/software(s):**

C++ with OpenMP/MPI

- **Key words :**

HPC, integrodifferential equation, dislocations

- **Thesis opportunity :**

Yes

- **Contact(s) :**

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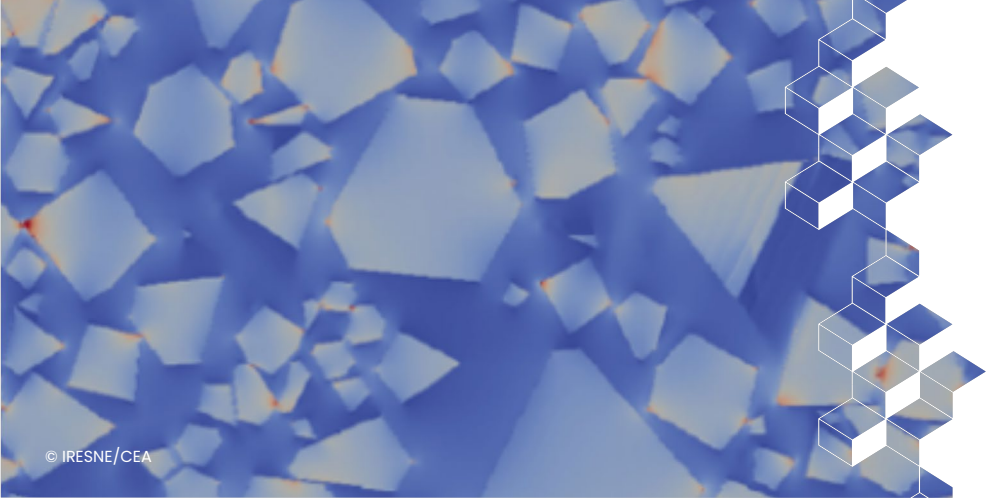

Numerical simulation of heat transfer in a microstructured heterogeneous material

DEC/SESC/LMCP

Heterogeneous materials with random microstructures, such as nuclear fuels, behave on the macroscopic scales as homogeneous materials [1], from the point of view of thermics or mechanics. This reduction of complexity by scale separation is highly valuable for modelling.

However, the homogenized properties (thermal conductivity, stiffness tensor) are not easily retrieved from the micro-structure description, notably when several physics are intertwined.

This internship aims at evaluating a numerical strategy for homogenization of a medium in which diffusion and radiative transfer phenomena are coupled. This strategy will be applied in order to evaluate effective properties of a fragmented fuel during an accident.

The internship is subdivided in two tasks :

- Participate and build a numerical tool for computing radiative heat transfer in a fragmented medium. This amounts to evaluating the radiative exchange between geometrical surfaces. Two options are possible : either the discrete transfer method, or Monte-Carlo methods [2].
- Use this tool and challenge the numerical strategy by quantifying its accuracy in various contexts.

This intership takes part to a current research project, which may yield a research article.

The candidate will have a deep understanding of scientific computing and thermal physics. A coding experience is required.

[1] G. Allaire. Shape optimization by the homogenization method. 2002.
[2] M. Modest and S. Mazumder. Radiative heat transfer. 2020

- **Desired schooling :**

M2 in physics or scientific computing

- **Duration :**

6 months

- **Method/software(s):**

Python and C++

- **Key words :**

Homogenization, thermal radiative transfer

- **Thesis opportunity :**

Yes, on a related topic

- **Contact(s) :**

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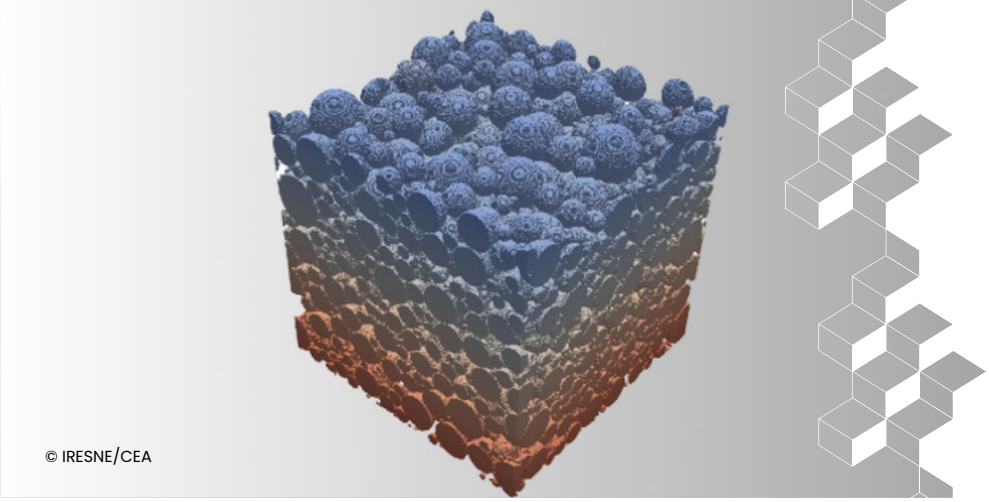

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Multi-scale simulation of thermal transferts in porous and granular media

DEC/SESC/LMCP

The study of the thermal behaviour of immersed granular media is of interest for a number of applications such as insulating materials, catalytic beds or even nuclear fuel combustion. In these applications, the material under consideration can present a porosity network at different scales (porosity between grain rings and porosity around grains).

The study of the thermal behaviour of immersed granular media is of interest for many applications, such as insulating materials, catalytic beds and nuclear fuel. In these applications, the material in question may have a network of porosity at different scales (porosity inside the grains and porosity around the grains).

Simulating and validating the thermal behaviour of granular media provides predictive tools for calculating the effective properties, such as thermal conductivity, of materials that are difficult to measure, and makes it easy to test the influence of microstructural parameters such as grain size or shape on the overall behaviour of the medium. To this end, a method combining the discrete element method (for mechanical properties) and the fast Fourier transform (for thermal properties) has been developed [1].

At the same time, a process of characterisation and modelling of materials simulating nuclear fuel was undertaken in order to better understand and validate the modelling of the thermal behaviour of these materials [2].

The aim of this work placement is to compare and validate the DEM/FFT method by comparing it with a series of experimental data and the analytical models developed previously. At the same time, the influence of various parameters such as the distribution of porosity between scales or the grain size distribution on the effective thermal conductivity of the granular medium will also be studied.

In practice, it will be necessary to familiarise oneself with the various calculation tools. Design the experimental plan for the simulations to be carried out. Run them, exploit and analyse the results.

This work placement is part of an ongoing research project. If successful, it could lead to the writing of a scientific article.
The successful candidate will have skills in thermodynamics, numerical simulation, programming and a taste for scientific research.

[1] T. Calvet, J. M. Vanson, R. Masson. A DEM/FFT approachto simulatethe effective thermal conductivityof granularmedia.International Journal of Thermal Sciences (2022)
[2] J. Letessier, A. E. Gheribi, J-M. Vanson, C. Duguay, F. Rigollet, N. Ehret, J. Vicente, J-L. Gardarein. Thermal transport porositymicrostructural characteristics: unpickingthe relationshipin ultra-porousα-Al2O3 powder. International Journal of Heatand Mass Transfer (2023)

- **Desired schooling :**

M2 in physics / thermal or scientific computation

- **Duration :**

6 months

- **Method/software(s):**

Python, C++, linux

- **Key words :**

Granular media, thermal transfer

- **Thesis opportunity :**

Yes

- **Contact(s) :**

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Department of Reactor Studies

The Department of Reactor Studies (DER) is an applied research unit with around 230 employees (80% of whom are researchers and engineers, and 20% technicians). The department hosts around 50 PhD students, post-docs and apprentices each year.

The DER's main activities involve :

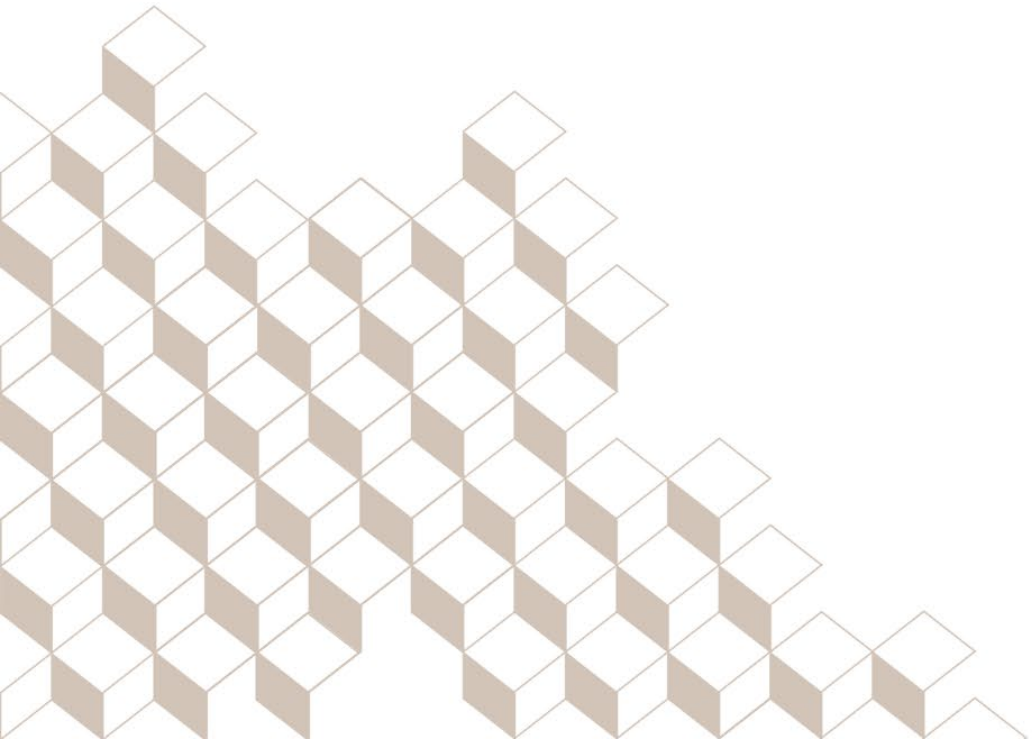
- pre-design of nuclear reactors and innovative energy systems, and support for current nuclear industry (FRAMATOME, EDF, ORANO, etc.),
- digital simulation,
- operating the CABRI experimental reactor and preparing the future Jules Horowitz Research Reactor (RJH),
- research reactor experimentation, innovative nuclear instruments.

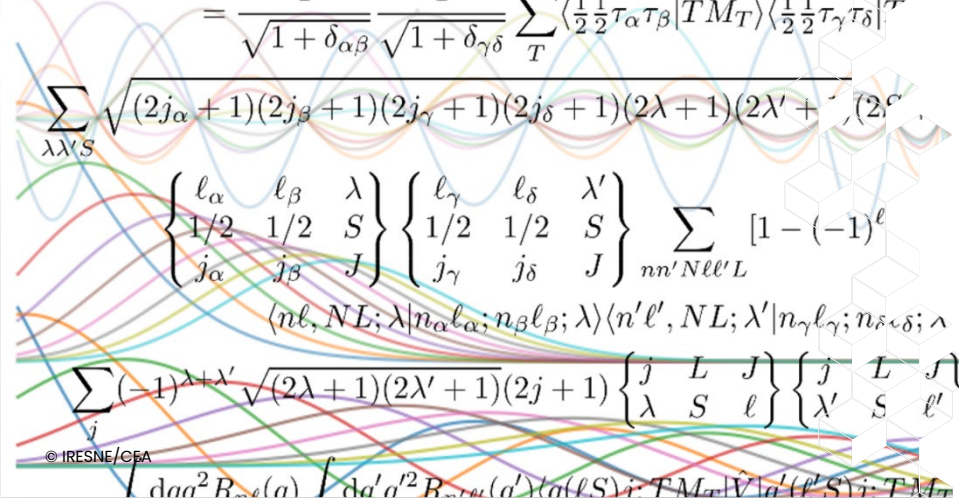
The DER comprises four units :

- Innovative Systems Research Unit (SESI),
- Experimental Physics, Safety Testing and Instrumentation Unit (SPESI),
- Reactor and Cycle Physics Unit (SPRC),
- Operating Jules Horowitz reactor unit (SERJH).

S P R C

Reactor and Cycle Physics Unit





Representation of the nucleon-nucleon interaction in mixed-basis Hilbert space

DER/SPRC/LEPh

Structure and reactions have remained separated fields of nuclear physics for a long time namely due to differing objectives. Continuous improvement of *ab initio* methods used in structure calculations open the possibility of new connection yet requiring modifications of numerical methods.

Several strategies exist to study nuclear structure, from legacy liquid-drop-based models to microscopic self-consistent mean-field (and beyond mean-field) approaches relying on various representations of the nucleon-nucleon interaction.

Phenomenological energy density functional (EDF) interactions – e.g. using Skyrme or Gogny forms – contains parameters adjusted on properties of nuclei spanning the whole chart of nuclides. *Ab initio* approaches however rely on bare nucleon-nucleon properties for instance on (n,p) or (p,p) scattering and deuteron properties. When more nucleons come into play, three-body interaction must be added to the two-body part. In *ab initio* approaches the three-body part remains adjusted on simple systems such as ^{3}He properties whereas EDF approaches introduce a local density-dependent term that breaks the symmetry of the many-body Hamiltonian.

The system relative coordinates between nucleons – the Jacobi coordinates – or the momentum space is well adapted for nucleon-nucleon scattering analysis therefore *ab initio* interactions are provided in such bases. For nuclear structure calculations, the interaction must however be transformed into a more global basis more closely related to the center-of-mass of the whole system.

The harmonic oscillator eigenfunctions have been a long-standing choice of basis for nuclear structure calculations. Their great asset is that they are solutions of a single-particle Schrödinger equation with a harmonic potential that can be chosen to approximate the mean-field. However because of the infinite asymptotic value of the harmonic potential, the structure results are poorly converging far from the system center-of-mass. This is a liability for exotic weakly bound systems and for further nucleon-nucleus scattering calculations that use these poorly converged results.

The selected candidate will have to study convergence properties of new (spherical) bases that he or she will have to define. Consistent orthogonal bases (harmonic oscillators, Bessel functions, etc.) will be first considered so that he or she will get familiar with the subject and the required tools. The second objective will consists in mixing these basis and to orthonormalize them so that the obtained basis could have good convergence far and close the system center-of-mass.

- **Desired schooling :**

Final year of MSc in nuclear physics, theoretical physics or condensed matter

- **Duration :**

6 months

- **Method/software(s):**

C/C++ or python programming skills, Unix environment

- **Key words :**

Theoretical nuclear physics, nuclear structure, *ab initio*

- **Thesis opportunity :**

yes

- **Contact(s) :**

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Nuclear Technology Department

The Nuclear Technology Department (DTN) is an R&D unit whose mission is to improve current nuclear reactor technology and develop that of future reactors by :

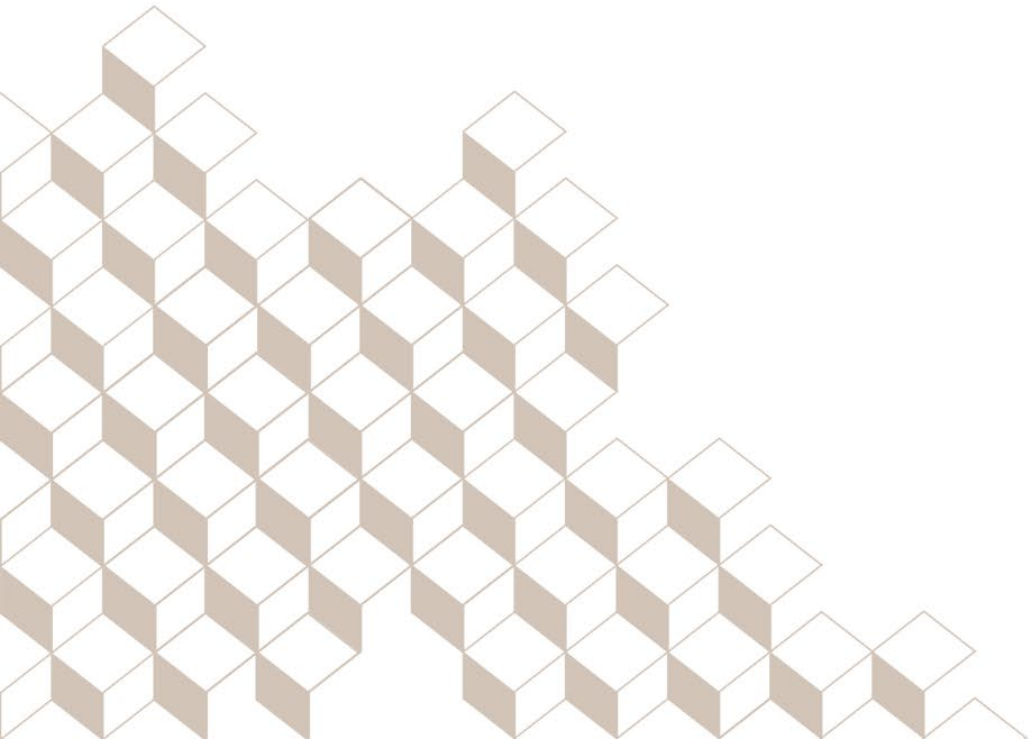
- studying, designing and carrying out qualification tests on reactor components (assemblies, devices, etc.),
- studying coolant behavior and performance,
- developing instrumentation for reactor monitoring, process control and nuclear measurement,
- modeling the transfer of radionuclides in the environment and in reactors,
- studying severe accidents.

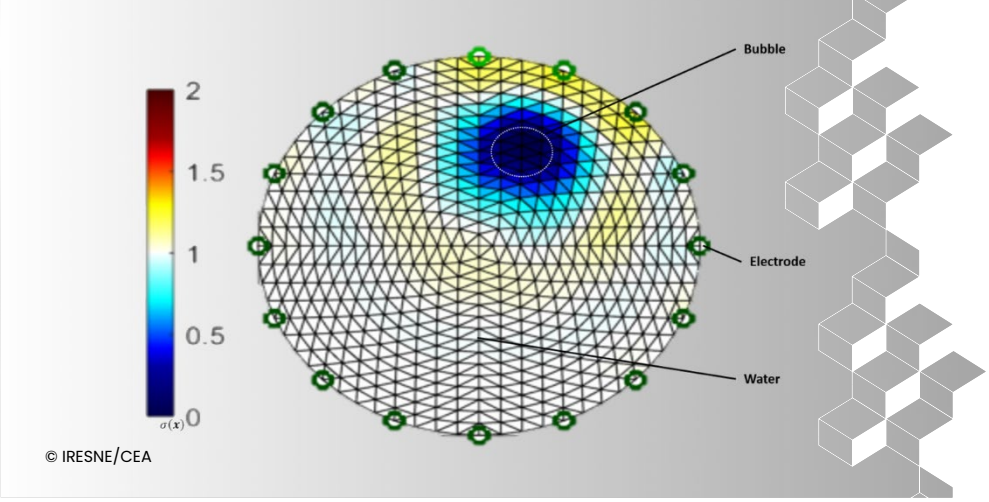
The DTN, which employs around 250 people (including 200 permanent staff, 30 PhD students, and post-docs, CDD OD or ATA, apprentices and trainees), is organized into two units:

- Transfer and Severe Accident Modelling Unit (SMTA),
- Component Technology and Processes unit (STCP).

STCP

Component Technology and Processes unit





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Generation of image reconstruction data for AI using a new electrical impedance tomography prototype

DTN/STCP/LISM

The CEA is developing instruments for the rapid detection of a possible accident in a nuclear reactor. In addition, estimating the void ratio and the distribution of phases in a flow is essential for understanding the evolution of an accident and controlling the risk of a boiling crisis in heat exchangers.

Electrical Impedance Tomography (EIT), a cousin of MRI and CT scans, is an innovative technology that allows the interior of a body to be imaged from measurements taken on the outside.

It involves placing electrodes around an object whose internal structure is to be measured. Electrical currents and potentials imposed and measured on these electrodes provide information about the impedance distribution according to Ohm's law.

For the time being, the models used have been able to roughly reproduce the shape of a large vacuum in the instrumented tube. In this internship, we want to improve the identification and quantification of foreign bodies.

To achieve this, the intern will first have to get to grips with the new prototype, for the experimental manipulations, as well as the algorithm developed in Python.

The idea is to identify the problems linked to image reconstruction in the code, and prepare several foreign body configurations in order to generate several data sets. The intern will also aim to gain an understanding of the artificial intelligence (AI) developed for image reconstruction.

Solving the inverse problem generally involves solving a poorly-conditioned matrix equation, so measurement uncertainties have a major impact on the result. A small part of the internship will therefore be to reduce all the measurement bias and noise as much as possible.

[1] DUPRE Antoine. Electrical impedance tomography for void fraction measurements of harsh two-phase flows: prototype development and reconstruction techniques. 2017. Thèse de doctorat. Ecole centrale de Marseille.

[2] DARNAJOU Mathieu, DUPRÉ Antoine, DANG Chunhui, et al. High Speed EIT with Multifrequency Excitation using FPGA and Response Analysis using FDM. IEEE Sensors Journal, 2020.

- **Desired schooling :**

Master 2
5th year of engineering school

- **Duration :**

6 months

- **Method/software(s):**

ITIE experimental prototype, Python, MATLAB, R

- **Key words :**

Electrical Impedance Tomography, Data processing, Artificial Intelligence, nuclear, start-up

- **Thesis opportunity :**

No

- **Contact(s) :**

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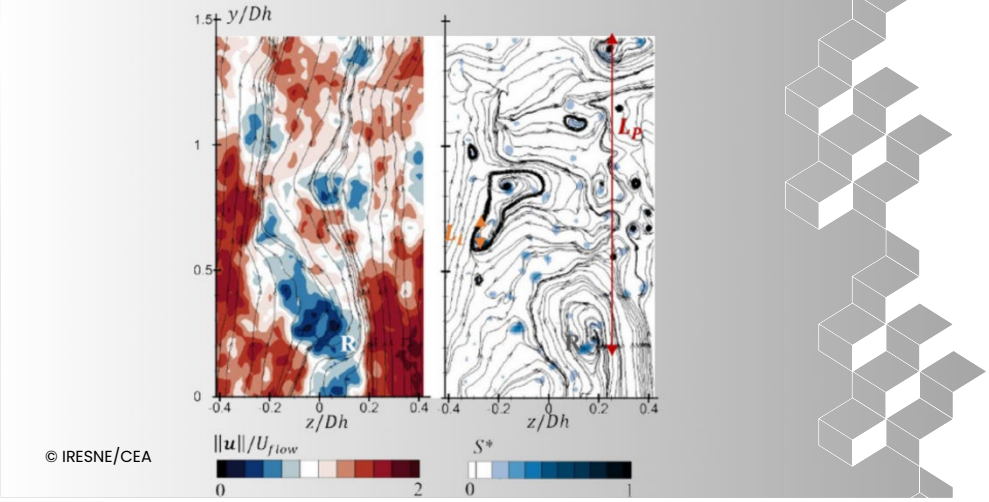

Experimental study of turbulent flow in fuel assembly bundles

DTN/STCP/LETH

Post–processing and analysis of flow measurements data (velocity fields and pressure) from a mock up representative of a sub-assembly

Fuel assemblies constitute the core of nuclear reactor core. Those small tubes attached together by grids are submitted to a strong turbulent flow. Amplified by grids, turbulent structures induce vibrations that can lead to fretting wear damages.

The topic of this internship is the study of the effect of different geometrical features of fuel assemblies on turbulent flow quantities, to understand their role in rod vibrations and grid-to-rod fretting. It could include the following activities (non-exhaustive list):

- brief literature review on turbulent flows in core fuel sub-assemblies;
- brief literature review on Particle Image Velocimetry (PIV) and Laser Doppler Velocimetry (LDV) post-processing and analysis;
- analysis of measurements data from previous experimental campaigns by relevant post-processing (Python or commercial tool);
- comparison with existing numerical results when possible.

The internship will include mostly analysis of experimental campaigns measurements, but the student could also be involved in the simulation work (CFD) done in the laboratory. It requires understanding of fundamentals of fluid mechanics (turbulent flows) and numerical methods (finite differences, Fourier transform…) and fluency in English (most of relevant literature on the topic is in English). Prior knowledge of turbulent flow in reactor core is not required.

[1] N. Turankok et al. *Exploration of frequencies peaks observed on local wall pressure measurements by time-resolved velocity field measurements in complex flows*. Experiment in fluids, 2021.

- **Desired schooling :**

MSc / Engineering school with major in fluid dynamics (final year student)

- **Duration :**

5 - 6 months

- **Method/software(s):**

literature review, measurements analysis and post processing (Python)

- **Key words :**

turbulent flow, reactor core, velocimetry, post-processing

- **Thesis opportunity :**

No

- **Contact(s) :**

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