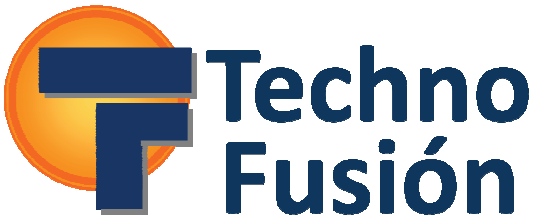

National Centre for Fusion Technologies

Scientific-Technical Report

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This document has been elaborated with the enthusiastic contribution of a large group of researchers from seven Universities and Research Centres. We are enormously grateful to them for their help and support during these past two years.

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Summary

The development of nuclear fusion is rapidly becoming a vital necessity in view of the continuing rise of the world's energy demand. Nuclear fusion offers a virtually endless source of energy that is both environmentally friendly and capable of meeting any foreseeable energy demand.

The progress of fusion constitutes one of the greatest technological challenges for humanity. Indeed, this field is one of the main areas of research of the European Union (EU), as was evident in June 2005, when the final agreement to construct ITER[1] (the *International Thermonuclear Experimental Reactor*) was signed, together with the USA, Russia, China, South Korea, Japan and India. ITER is an experimental reactor intended to demonstrate the scientific viability of fusion.

As the design of ITER is already defined, over the next 20 to 30 years the main focus will be on the development of technological components for future commercial reactors, rather than on basic plasma physics. The most important challenges for fusion research are the selection, development and testing of materials and the various elements for reactors, together with the design of energy extraction systems and tritium production methods.

At present, Spain has a unique opportunity to be at the forefront of this new technological field in Europe. However, there is a need for new facilities to simulate the extreme conditions to which materials and components will be exposed inside a fusion reactor.

The project outlined in this report describes the construction of a singular scientific and technological facility (the National Centre for Fusion Technologies -*TechnoFusión*) in the Madrid region, to create the infrastructure required to develop the technologies needed in future commercial fusion reactors, and to assure the participation of Spanish research groups and companies.

The Spanish scientific community has achieved an international recognition in the science and technology areas needed for the success of this ambitious project, as is evident from the results obtained by Spanish researchers in the fusion field over the past few decades. *TechnoFusión* intends to take advantage of the existing expertise of university research groups, public research institutions (*Organismo Público de Investigación, OPI*) and private companies. The performance of materials and components under the extreme conditions of a fusion reactor is largely unknown, and this is precisely what *TechoFusión* intends to explore. For this purpose, facilities are required for the manufacture, testing and analysis of critical materials. Additional resources are planned to develop and exploit numerical codes for the simulation of

[1] ITER (originally the International Thermonuclear Experimental Reactor) is an international tokamak (magnetic confinement fusion) research/engineering project being built in Cadarache, France.

materials in special environments, to develop remote handling technologies and other areas related to the management of liquid metals.

In summary, *TechnoFusión* focus is the creation of infrastructures for the following research areas: 1) material production and processing, 2) material irradiation, 3) plasma-wall interaction (thermal loads and the mechanism of atomic damage), 4) liquid metal technologies, 5) material characterization techniques, 6) remote handling technologies and 7) computer simulation.

Therefore, *TechnoFusión* Scientific-Technical Facility will thus consist of a complex of seven large research areas, many of which are unique in the world, with the following main technical objectives:

1) *Material production and processing*. There are still some uncertainties about the materials that will be used to construct future fusion reactors, partly because it has not yet been possible to reproduce the extreme conditions to which such materials will be subjected. Therefore, it is of utmost importance to dispose of installations capable of manufacturing new materials on a semi-industrial scale and fabricating prototypes. Top priority materials include metals such as reinforced low activation ODS type steels (*Oxide Dispersion Strengthened steels*) and tungsten alloys. To manufacture such materials, equipment is required that currently is scarce or inexistent in Spain, such as a *Vacuum Induction Melting Furnace* (VIM), a *Hot Isostatic Pressing Furnace* (HIP), a Furnace for Sintering assisted by a Pulsed Plasma Current (*Spark Plasma Sintering*, SPS), or a *Vacuum Plasma Spraying* (VPS).

2) *Material Irradiation*. Even though the exact reactor conditions are only reproduced inside a reactor, it is possible to simulate the effects of neutrons and gamma radiation on materials by irradiating by ion and electron accelerators.

The effect of neutronic radiation will be characterized by combining three ion accelerators: one light ion accelerator of the tandem type for irradiating with He, with an energy of 6 MV, one light ion accelerator of the tandem type for irradiating with H (or D), with an energy of 5-6 MV, and a heavy ion accelerator of the cyclotron type, with k = 110, to implant heavy ions (Fe, W, Si, C) or high energy protons.

Additionally, a high magnetic field, between 5 and 10 T, must be incorporated into this facility in order to study the simultaneous effect of radiation and magnetic fields on materials.

The effects of ionizing *gamma* radiation will be studied using a *Rhodotron®* electron accelerator with a fixed energy of 10 MeV that will be shared with other *TechnoFusión* facilities.

3) *Plasma-wall interaction*. Inside a fusion reactor, some materials will not be subjected only to radiation, but also to enormous heat loads in the case of plasma disruptions. In view of this, both: i) stationary conditions due to the intrinsic reactor properties: high density, low temperature and high power and ii) violent transient events (called ELMs in plasma physics literature) must be reproduced. Therefore, it is essential to dispose of a device (which it will be called “plasma gun”) to study plasma-material interactions simultaneously in steady state and transient regimes, thereby allowing an analysis of the modification of the materials and their properties in fusion reactors.

The mentioned plasma gun would consist of two main elements: i) a linear plasma device capable of generating hydrogen plasmas with steady state particle fluxes of up to 10^{24} $m^{-2}s^{-1}$ (i.e., of the order of the expected ITER fluxes) and impact energies in the range of 1-10 eV, and ii) a device of the quasi-stationary plasma accelerators (*QSPA*) type, providing pulses lasting 0.1-1.0 ms and energy fluxes in the 0.1-20 MJm^{-2} range, in a longitudinal magnetic field of the order of 1 T or greater.

These devices are connected by a common vacuum chamber, allowing the exchange of samples, and their simultaneous or consecutive exposure to the steady state and transient plasma flows under controlled conditions. Both devices will operate with hydrogen, deuterium, helium, and argon.

4) *Liquid metal technologies*. A number of, ITER, DEMO (*DEMOstration Fusion Power Reactor*)[2], and IFMIF (*International Fusion Materials Irradiation Facility*)[3] components will use liquid metals as refrigerants, tritium generators, neutron reproducers, moderators, etc., all of them under extreme conditions. Therefore, these applications need further research to be finally implemented in such installations.

The basic working scheme for this Facility in *TechnoFusión* is an arrangement of two liquid lithium loops, one of them coupled to the *Rhodotron®* electron accelerator to investigate the effects of gamma radiation on different conditions of the liquid lithium.

The main goals of this Facility are the studies of i) the free surface of liquid metals under conditions of internal energy deposition, and ii) the compatibility of structural materials and liquid metals in the presence of radiation. In addition, it will be possible to study the influence of magnetic fields on the cited phenomena as well as the development of methods for i) purification of liquid metals, ii) enrichment of lithium, iii) extraction of tritium, and iv) development of safety protocols for liquid metal handling.

5) *Characterization techniques*. Ambitious and well-understood research requires an accurate knowledge of the materials under study. Therefore, a range of techniques to characterize them under different situations is a key element in the global scheme of *TechnoFusión*. These techniques include mechanical testing (creep, nanoindentation, fatigue, etc.), compositional analysis (Secondary Ion Mass Spectrometry and Atomic Probe Tomography), and structural characterization (Energy Filtered Transmission Electron Microscopy, X-Ray Diffraction), as well as a number of material processing techniques (Focused Ion Beam Systems coupled to a Scanning Electron Microscope). Additional systems will be used to characterize physical properties (electrical, dielectric, optical, etc.).

Some of the above-mentioned techniques will be implemented to test the materials either in-beam –while being irradiating— or *in-situ*, inside the lithium loop. Needless to say, these techniques can also be performed before and after irradiation or before and after experiencing any other physical or chemical processes.

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[2] DEMO (DEMOnstration Power Plant) is a proposed nuclear fusion power plant that is intended to build upon the expected success of the ITER experimental nuclear fusion reactor.

[3] IFMIF is a planned high-intensity neutron reactor whose spectrum should be equivalent to that of a fusion reactor. The final design comprises two deuteron accelerators impinging on a liquid lithium target to generate nuclear stripping reactions to provide the desired neutron spectrum

6) ***Remote handling technologies***. The conditions inside a fusion reactor are incompatible with a manual repair or replacement of parts. Therefore remote handling is indispensable. New robotic techniques, compatible with such hostile conditions, need to be developed; while existing techniques need certification in order to be applied at installations such as ITER or IFMIF.

TechnoFusión Facility will contribute to this knowledge with: i) a large installation for the prototypes manipulation such as: *Diagnostic Port Plug* of ITER, *Test Blanket Modules* of ITER and Modules of irradiation of IFMIF, and ii) an Irradiated Room coupled to the electron accelerator –*Rhodotron*®— in order to carry out validation, certification and characterization of remote handling tools and machines in an uniform ionizing field equivalent to ITER-DEMO trying to simulate the fusion reactor environment.

7) ***Computer simulation***. To study conditions that cannot be reproduced experimentally and to accelerate the development of novel systems for a future commercial fusion power plant, *TechnoFusión* will stimulate an ambitious programme of computer simulations, combining existing experience in the fusion field with resources from the National Supercomputation Network[4]. The goals include the implementation of the global simulation of a commercial fusion reactor, the interpretation of results, the validation of numerical tools, and the development of new tools. Another indispensable goal is the creation of a data acquisition system and the visualisation of results.

Based on the existing experience of research groups at Universities, Public Research Organisations and company research departments, *TechnoFusión* proposes the development of a large scientific infrastructure in order to make a significant contribution to the development of new technologies needed for the construction of commercial fusion reactors. The project described here will permit the generation of highly relevant technological knowledge for all types of fusion reactors, irrespective of the underlying concept (magnetic or inertial confinement).

The goal of TechnoFusión is to bring together sufficient human and material resources to contribute significantly to the development of a safe, clean, and inexhaustible source of energy for future generations.

[4] http://www.bsc.es/index.php. September 2009.

10. Computer Simulation

10.1. Introduction

The interaction between theory, including both speculations and logical demonstrations, and direct experimental observation lies at the basis of modern science. Theory, developed to a high degree of complexity with the help of ever more powerful mathematics, has allowed explaining many features of nature, and has often produced predictions that have only later been confirmed by experiment. The maximum attainable level of knowledge is obtained when models reproducibly predict events, given the same initial conditions.

The translation of theoretical models into computational models has made it possible to perform detailed simulations of physical phenomena with ever increasing accuracy. Today, the importance of computer simulation as a complement to experimentation is generally accepted. Simulation is used in research to generate new knowledge, and in engineering to facilitate the design of new technological facilities based on existing knowledge.

There is a wide international (and, of course, European) consensus that the design of components for facilities like ITER, IFMIF, DEMO, etc., requires computer simulations of both physics and engineering issues, alongside the appropriate experimental validation of the theories on which these simulations are based. In some cases, these computational models cover disparate spatial and temporal scales, so that Multiscale Models are required. Such models call for advanced programming knowledge, and require extensive computing resources and special visualisation tools. These resources are generally not available to every research group, making it difficult for a researcher without previous experience in this field to take full advantage of the undisputed potential of this technology. The **Computer Simulation Facility (CS)** of *TechnoFusión* aims to offer to research groups and companies expert support (including both personnel and the necessary tools), so that a complex Multiscale Simulation task can be undertaken in a relatively short period of time, in the framework of a multidisciplinary collaboration between the Facility and the external user. The proposal does not contemplate the possibility of installing a large computer on the premises of the centre; instead, use will be made of existing national and international computer facilities.

The main field of application of the CS Facility can be subdivided in two broad categories: i) problems related with engineering calculations needed for the detailed design of complex facilities (sometimes consisting of millions of components), and ii) those associated with physical phenomena taking place in a fusion reactor.

In Spain, ample experience in this field is available. However, this knowledge is dispersed among many universities (UPM, UA, UNED, UAM, UAB, UV,etc.) and research centres (CSIC, CIEMAT, etc.), so that the creation of a consolidated and integrated working group is desirable in order to centralise the various tools and make them available to potential users interested in their application to different aspects of fusion technology.

10.2. Objectives

Three major objectives are considered. An immediate objective of the Laboratory will be to undertake the computer simulation of all the components of the *TechnoFusión* (TF) facilities. This task will tackle outstanding challenges in the field of simulation. The second objective is of fundamental importance in medium and long term and involves creating and maintaining a team capable of carrying out computer simulation work as needed in the design of the installations of ITER, DEMO, the Commercial Fusion Reactor, and the supporting IFMIF irradiation facility. The third objective of the laboratory is to provide the required data handling capacity (data acquisition, storage, visualization/interpretation) as data are produced by the experiments performed at the *TechnoFusión* facilities; as well as the software needed to control the operation of the mentioned facilities.

In order to achieve the abovementioned objectives, the following activities must be undertaken:

I) To obtain and/or develop and/or adapt the required (adequately validated) computational methodology needed to assure that the design of the *TechnoFusión* facilities (accelerators, the lithium loop, etc) matches to the requirements for the operation of such facilities.

II) To obtain and/or develop and/or adapt the required (adequately validated) computational methodology needed to assure that the design of the *TechnoFusión* facilities (accelerators, the lithium loop, etc) matches to the requirements concerning radiological protection and safety.

III) To obtain and/or develop and/or adapt the required (adequately validated) computational methodology needed to manage the data (obtained from the experiments), including control systems for the *TechnoFusión* facilities.

IV) Establish sufficient simulation capacity to be able to handle the technologies to be incorporated in irradiation facilities such as IFMIF, based on high intensity accelerators.

V) Establish sufficient simulation capacity to be able to handle the technologies to be incorporated in the design of ITER, DEMO, and a Commercial Reactor.

In many areas of fusion technology, computer simulation can play a significant role. Some of the foremost issues are:

- The identification of particles and radiation emitted from the plasma, and their interaction with matter.
- The effect of radiation on materials.
- The interaction of neutrons with the blanket, requiring a description of energy deposition and the process of tritium generation.

- Knowledge of the fluid dynamics of the coolants (needed for energy extraction), and their effect on system components (corrosion, diffusion, the generation of impurities, etc.)

- The identification of the pathways for the release of tritium and other activated elements.

- Radiation transport, activation and dose calculations (prompt and residual), with implications for safety and the environment (the classification of plant materials, the definition of management, calculations of shielding, etc.)

- The interaction of the plasma with the first wall and its effects on the plasma and the properties of the material.

- Thermo mechanical calculations in complex components for design validation.

The establishment of the CS Facility is essential for the *TechnoFusión* facility itself, and in addition it is considered important to have an expert team at our disposal capable of executing and distributing the required computational work (including theoretical developments, when needed) regarding the various aspects associated with both ITER and future commercial reactors. Additionally, the CS Facility should have the capacity of dealing with the processing (and visualisation) needs that will arise once the experimental data start flowing in, both regarding equipment and personnel.

In the framework of the research and development needed for a future fusion reactor power plant, some well-defined areas exist which will be described next. Once the fusion reaction is initiated, energy is liberated in the form of neutrons, charged particles and electromagnetic radiation. Each of these particles interacts with the environment, thus allowing both the generation of enthalpy, to be extracted by means of a circulating coolant, and of tritium, required for the fuel cycle. But the liberated particles and energy are also responsible for problems associated with very large temperature gradients and damage caused to the crystalline or amorphous structures of the materials employed, affecting their operational lifespan, and causing the activation of the material. Given the fusion power source and a particular reactor design, the study of the following issues is therefore needed (to be modified iteratively):

- Radiation flux and fluency as a function of space (3D) and time:
  - Atomic and nuclear data.
  - Particle transport and interaction mechanisms (neutrons, charged particles and radiation).
- Heat deposition and its consequences, and heat extraction from the reactor:
  - Energy deposition methods.
  - Computational fluid dynamics with high spatial and temporal resolution.

- Thermo mechanical models.

- The effect of neutron irradiation on materials:
  - Multiscale simulation of the irradiation of materials.

- The consequences of tritium management:
  - Diffusion in material models.
  - Paths for tritium release from the system.
  - The evaluation of atmospheric dispersion and its consequences.

- The effect of radiation and activation induced by neutrons and other types of radiation as a function of radioprotection measures:
  - Highly detailed inventory models capable of simulating operational scenarios characterized by different types of radiation and energy spectra, with time dependence.
  - Computational methods for the prediction of the prompt and residual dose rate.
  - The generation, assessment and classification of radioactive waste.

- The implications of a given Plant design:
  - Plant engineering models capable of simulating the energy conversion system, critical points, and the operational situations and accidents that could occur in the Plant (safety issues).

In this preliminary stage, the aim is to identify the models already available for each of these proposed areas, or at least easy to obtain, and their suitability for solving the problems raised in the study of fusion facilities (ITER, IFMIF, etc.), as well as their computational requirements. This pioneering integral approach to knowledge is crucial for the conception of this facility of *TechnoFusión*.

The experimental facilities of *TechnoFusión* will require a suitable system for the acquisition, control, visualization and analysis of data:

- The Area for Visualization and Analysis will provide:
  - Support for data acquisition.
  - Support for data storage and backup.
  - Support for data access.

- Many experiments will require real-time complex control systems (cf. the experience at TJ-II)
- Centralization to simplify quality control.
- Both experiment and simulation require new analysis techniques due to:
  - The data volume (increasing with time).
  - The complexity of the systems analyzed.

- The Area for Visualization and Analysis will allow:
  - Extracting the maximum amount of information possible.
  - Presenting this information in a useful and attractive manner

In addition, the Computer Simulation Facility of *TechnoFusión* should include computational support, in order to provide the following services:

- Acquisition
- Maintenance
- Support
- Training
- Networking

10.3. Resources

The CS Facility will require ample resources (both personnel and infrastructure) in order to tackle the full computer simulation of the components of the facilities and their dynamical behaviour in a future fusion reactor. Therefore, the proposed CS Facility will cover:

- Simulation Models to determination particle fluxes (neutrons, charged particles and radiation) towards the system components. For this purpose, 3D MonteCarlo and Discrete Ordinates codes will be used, such as recent versions of MCNP or ATILA (SN). Also, tools will be developed to translate the graphical description of the plant (usually supplied in CATIA format, as is the case with ITER, for example) to the required input files for these codes.

- Simulation Models for the interaction of charged particles with matter, including phenomena like sputtering and wall erosion, based on basic codes like TRIM and

SRIM, as well as more detailed codes, involving Binary Collisions or Molecular Dynamics, and appropriately coupled to codes for the simulation of the plasma from an electromagnetic point of view. This particular aspect is crucial for the technological description of First Wall phenomena.

- Liquid metal fluid dynamics codes, including codes like FLUENT, STAR-CD or CFX, which can be used for the design of the blanket and the evaluation of its reliability for DEMO, within the framework of ITER.

- Structural simulation models based on programs like CATIA or ANSYS.

- Simulation models for the irradiation damage of materials: metals, ceramics and insulators. With this aim, Multiscale Simulation schemes will be implemented, including:

    - Ab initio quantum-mechanical calculations, to be developed alongside codes like SIESTA (UAM) and VASP.

    - Molecular Dynamics codes, including MDCASK and more flexible codes incorporating fundamental interatomic potentials, some of which are still under development (even for metals), and which ideally should be capable of describing displacement cascades and the basic mechanisms associated with irradiation damage.

    - Defect diffusion, based on Kinetic MonteCarlo or Rate Theory techniques, incorporating recent developments with respect to parallelization (as with BIGMAC), and providing a reliable description of long-term irradiation effects.

    - Dislocation Dynamics (DD), including the development of models suitable for materials with a variety of structures (fcc, bcc and others) on the basis of codes like DD·D or PARADIS, and the incorporation of dislocation and defect interactions.

    - Finite element models that allow calculating the macroscopic properties on the basis of parameters that have been obtained from the simulation of underlying processes.

- Simulation models for dose rate calculations (radioprotection)

    - Prompt dose: Computed on the basis of the most recent transport codes and databases; or by selection and integration of the appropriate computational elements. For many applications, it will be necessary to develop a proper methodology. A key aspect of this process is that the methodology must be validated for all the proposed *TechnoFusión* applications.
    - Residual dose: The ACAB activation code will be one of the main computational tools. ACAB incorporates the quantification of material activation by neutrons, radiation, and charged particles for any energy spectrum and irradiation-cooling scenario. Quantities related to activation are

predicted along with an estimation of the uncertainty due to the error in the cross sections used. Responses provided by the code allow radioprotection-safety assessments and the classification of irradiated materials from the perspective of their post-irradiation management (hands-on management or recycling, surface burial, declassification, etc.).

Below, it is discussed some of the salient features of *TechnoFusión* in more detail, due to their importance for the development of fusion facilities and the interpretation and analysis of results.

10.3.1. Safety Area

The numerical evaluation of the consequences of safety hazards, by means of computer simulations, is considered fundamental for the design of a fusion facility and for the determination of its operational parameters. The main requirement would be to avoid the need for evacuation in the worst-case accident scenario. The aim of the safety analysis is to predict the impact on public health of an accident. For this purpose, three basic tasks are contemplated:

- A calculation of the radioactive inventory.
- The determination of the source term of accidental emissions.
- The evaluation of effects or final responses.

Possible tools for carrying out these tasks are:

i) **The calculation of the radioactive inventory:** the ACAB, FISPACT and ORIGEN codes. ACAB allows calculating the evolution of the isotopic inventory after material activation by neutrons, charged particles, or photons. Quite general irradiation/cooling regimes can be modelled as well.

ii) **The determination of the source term**, indicative of the radioactivity released into the environment: one must characterize accident scenarios in a sufficiently detailed manner, and perform the analysis thereof using thermohydraulic and heat transfer codes. Relevant key tools are the heat transfer code CHEMCON and the thermohydraulics code MELCOR. CHEMCON is used to simulate the evolution of the temperature due to decay heat and oxidation reactions. The calculated record of temperature vs. time then allows identifying the source term. The latter is input to the MELCOR code, which simulates the associated thermohydraulic phenomena, including the physics and dispersion of aerosols and the release of radioactive products. Tritium migration, in turn, can be simulated using the TMAP code (*Tritium Migration Analysis Program*)

iii) **Evaluation of consequences:** a method is needed to generate the DCF (Dose conversion factor, expressed in Sievert per released Bequerelium, Sv/Bq) for the released radionuclides, which, in turn, allows estimating the doses and health effects of the emission. These DCF libraries are obtained through codes like MACCS and their associated data libraries.

10.3.2. Waste Management Area

A widely accepted requirement for waste management in fusion facilities is to avoid deep geological storage of radioactive waste. ACAB and FISPACT allow estimating the generated radioactive inventory and evaluating its classification in the framework of given waste management criteria/strategies: surface burial, recycling by nuclear industry and declassification.

10.3.3. Uncertainties

The evaluation of a nuclear system depends on the ability to understand the physics underlying the whole process, from the fundamental physics of the nuclear reactions to neutronic, thermomechanic and thermohydraulic responses, material science, etc. Energy production, irradiation damage, radioactivity, decay heat and other related magnitudes are the result of the interaction between particles and nuclei. Therefore, in order to improve the description of the macroscopic effects of these mechanisms, an accurate knowledge of these quantities is required.

Therefore, in the state of the art of the nuclear system simulations, the uncertainties of nuclear data play an important role. The ultimate goal is to estimate the uncertainties propagation across all calculation steps, from the generation of nuclear data and its processing to the prediction of the radioactive inventory, particle transport, thermal and thermohydraulic analyses, etc. Through the implementation of, for example, first order perturbation and MonteCarlo techniques, it is possible to perform a complete sensitivity/uncertainty analysis at every stage.

10.3.4. Radiological Protection Area

In this area, the basic analysis tools are transport codes (and cross sections and/or models used to describe nuclear interactions), able to deal with different types of radiation and to determine the spatial distribution of the source terms and fluxes. Once the particle fluency has been determined, it is possible to obtain a radiological classification by means of the fluency to dose conversion factors, which are dependent on the energy and type of particle.

Transport codes of reference are:

- **MCNPX**: A MonteCarlo method transport code. It allows modelling the transport of neutrons, photons and charged particles. Version 2.5 computes the transport of light particles only (electrons, protons, deuterons, tritons, alpha particles). Version 2.6, still under development and not yet officially released, incorporates improved nuclear models for the determination of the reaction cross sections. It will also allow modelling the transport of heavy ions.

- **PHITS**: A MonteCarlo method transport code. It allows modelling the transport of neutrons, photons and light and heavy charged particles. Cross sections for nuclear reactions are calculated from nuclear models incorporated in the code.

- **FLUKA**: This is a general purpose MonteCarlo simulation tool for the calculation of particle transport and interactions with matter. It can simulate the interaction and propagation of about 60 different particles in matter with high accuracy. The top priority for the design and development of FLUKA has always been the implementation and improvement of sound and modern physical models.

In the case of ion transport, it will be crucial to estimate the corresponding material implantation and diffusion levels. Some selected codes are:

- **SRIM**: A MonteCarlo ion transport code. This code simulates the transport of charged particles, taking account of the dispersion processes only, due to either the electrostatic stopping power or nuclear interactions. It does not consider any nuclear reactions that could take place during particle transport. Its main use is the determination of implantation and energy deposition profiles in matter.

- **TMAP**: A deterministic diffusion code. This is a 1D code that allows establishing the evolution of concentration profiles for implanted ions. Its main purpose is the determination of the number of ions that have entered and left the material. The code is suited for the calculation of tritium diffusion in a material and its eventual release from it, and for estimating the total accumulation of ions inside the material, leading to D-D nuclear reactions as a consequence of high-energy deuterons originating from the accelerator.

Since some of the *TechnoFusión* laboratories will be radioactive installations, their design and the preparation of licensing documents will require prior studies on radiation protection and safety. Therefore, this will be a major task during the first phase of the computational laboratory. Currently, no reliable computational methodology exists to predict prompt and residual dose rates corresponding to the accelerators and associated irradiation modules of *TechnoFusión* (and other irradiation facilities driven by accelerators, such as IFIMF-EVEDA). Thus, one of the key objectives is to develop and implement a computational methodology capable of addressing the needs of *TechnoFusión* regarding radiation protection, and to carry out the evaluation and validation of all its computational elements. A secondary objective will be to apply this methodology to the design and operation of accelerators and irradiation modules, in order to show that an adequate solution has been achieved for all potential radioprotection issues.

10.3.5. Nuclear data analysis: the identification of potential requirements

(I) Nuclear data libraries

- *Neutron, proton and deuteron transport libraries.* Until recently, the FENDL-2.1 library has been adequate for calculations related to fusion facilities (ITER). However, the design of novel neutron sources such as IFMIF will require particle transport data for energies above 20 MeV (IFMIF will even require data up to 60 MeV). The range of data with potential fusion applications extends to even higher energies, namely up to 150 MeV. In order to develop such data libraries, codes will be needed in order to predict the effects of this type of nuclear reactions, in combination with experimental data contained in the EXFOR library. Thus, it is considered essential to develop tools to update existing libraries and extend their range to higher energies. In addition, the libraries must be completed with information on the covariance, derived from theoretical models or experimental results. And finally, programs or procedures need to be developed that are suitable for generating specific libraries through the use of NOY.

- *Neutron, proton and deuteron activation libraries.* The most complete activation library to date is EAF2007, including sub-libraries for neutrons, protons, deuterons and disintegration processes. Proper tools should be developed in order to transform these libraries into the ENDF format, and include the uncertainties or covariance values of the activation reactions for a broad range of energies.

- *Experimental activities.* Studying and evaluating existing experimental data, and identifying the need for additional experimental data.

(II) Codes for cross section generation

In order to estimate the probability of any nuclear reaction, transport codes like MCNPX or PHITS either use cross section libraries or built-in nuclear models. In the latter case, it has been noted that results can vary significantly from one code to the next, due to the specific estimations of cross sections included in each model.

Thus, one can conclude that it is essential to benchmark the cross sections used in the codes against experimental or simulated values.

- *Talys 1.0, EMPIRE-II 2.18.* These codes calculate nuclear reaction cross sections using several nuclear models, such as the optic model, direct reactions, the compound nucleus model, the pre-equilibrium model, etc. These codes produce cross sections for a particular reaction or for the production of a given particle (neutron, proton, etc.), and determine the differential cross section. These cross sections should be benchmarked against the experimental or simulated data contained in libraries like EXFOR.

10.3.6. Thermo mechanical simulation codes

Generally, these codes are finite element codes. Simulation codes designed in the past five years tend to unify the mechanical and thermohydraulic calculations, so that the cooling properties of a body and its mechanical stress distribution can be analyzed simultaneously. Prominent examples of this type of code are those developed by companies like START-CD and ANSYS.

- *The ANSYS code* is a widely used calculation platform that unifies modules originating from several independent codes. Each of these modules allows solving a clearly defined branch of physical problems. Below, a brief description of the various computational modules and their potential application is given:
  - *Ansys Fatigue Module:* starting from an ANSYS standard geometry, this module allows performing fatigue calculations in the following conditions: constant amplitude and linear and non-linear loads.
  - *Ansys Mechanical Module:* this is the module upon which the rest of the code rests. It allows simulating a solid using finite element analysis. It is possible to solve the following physical processes in a coupled way: acoustic, piezoelectric, thermomechanical and thermoelectric analysis, electromagnetic fields in the high and low frequency range, and the mechanical analysis of an elastic solid.
  - *AutoRegas:* is a DCF module developed to solve gas explosion problems in pipes and confinement chambers with complex geometries.
  - *CFX*: is a DCF module that is completely coupled to the generic meshing of ANSYS. By using these meshes it can interact with the mechanical module without interpolating on the solid surfaces. It also allows performing the following simulations: turbulence, chemical reactions, heat and radiation transfer, and multiphase problems.
  - *Fluent:* is a DCF code developed independently from all other ANSYS modules. The company owning the code has recently been acquired by ANSYS, so one can assume that this code will be fully integrated in the near future. Presently, Fluent is a separate program, which can read the ANSYS mesh and export its calculations in generic ANSYS format. It is able to solve the following problems: turbulence, acoustics, chemical reactions, heat and radiation transfer, multiphase problems, and magnetohydrodynamics.
  - *Polyflow:* is an ANSYS module to simulate viscoelastic materials. It allows simulating extrusion, blow moulding and similar shaping processes.
  - *Tgrid y Gambit:* are two generic mesh generators supplied with the ANSYS package. In principle, both are able to import specialized CAD geometries and generate a mesh of hexahedrons and tetrahedrons.

- *The STARCT-CD code* is a general-purpose finite element program, capable of simulating both solids (thermomechanics and heat transfer) and fluids on the same mesh. It allows solving the following problems: thermal analysis, mechanical analysis, chemical reactions, free surface problems, multiphase problems and turbulence.

- *The Open Foam code* is an open source, generic finite element code. It disposes of a number of pre-programmed modules, capable of solving generic problems, such as thermal analysis, turbulence, multiphase, and free surface problems, mechanical analysis, magnetohydrodynamics and electromagnetism, and combustion reactions. In contrast with the codes mentioned above, it is still in a relatively early development stage, and has a poor graphic interface, so that users need to have a thorough background in C++ programming. If this is the case, the addition of new models is quite straightforward, so the code can be applied to almost any subject. The only limitation of the code is that it can only handle a single control volume having the same equations on every node, so that it is not possible to simulate solids and liquids simultaneously.

- *The Flow3D code* is a FDC code with features similar those of CFX, Fluent or Start-CD. Outstanding features include the modelling of turbulence, heat and radiation transfer, acoustics, phase transitions, multiphase problems, free surface problems, mechanical stresses in solids, electro-osmosis, dielectrics, joule heating and viscoelastic solids.

10.3.7. Transitory thermal analysis

Transitory thermal analysis codes (like Relap) are an essential tool for the analysis of the behaviour of complex facilities during thermal transients. Even if the objectives of *TechnoFusión* do not include detailed full plant studies, these tools could nevertheless be very useful for the analysis of experimental facilities like the liquid lithium loop of *TechnoFusión*.

- *Relap5* is the latest branch of a family of codes for analyzing transients in nuclear plants, developed by the government of the UE over the past 30 years. In the last few years, it has been applied to the study of a design basis accident in the AP600 reactor series. Some salient features are: thermohydraulic models, 1D for loops, 2D for complex structures, heat transfer, models for complex systems (vessel, steam generators...), 1D and 2D heat conduction in complex structures, models for generic components like pumps, valves, electric elements and potential implementations of control systems in the module. A drawback is that the models for fluids other than water are unsatisfactory, making it impossible to analyze liquid metal loops.

- *Melcor* is a program developed by *Sandia National Laboratories* and financed by U.S.N.R.C for the study of severe nuclear plant accidents. Some salient features are: thermohydraulic models, heat transfer, in-fuel chemical reactions, hydrogen generation both inside and outside the vessel, and the generation and diffusion of radioactive aerosols.

10.3.8. The evaluation of the environmental impact of an atmospheric release

When a future fusion reactor suffers an accident, gases are released into the atmosphere, including tritium, and these will be dispersed in the atmosphere. The evolution of this dispersion depends on the atmospheric conditions in the area surrounding the discharge. The empirical model used to evaluate the resulting environmental impact is based on the Gaussian equation and a straight plume trajectory from the time of release onward. It is a diffusion model in an ideal atmosphere, yielding a normal distribution in all directions around the central axis of the radioactive plume. To improve the realism of this model, more information on the behaviour of tritium in the environment of a nuclear fusion facility should be added.

Tritium will primarily be released in the form of gas, i.e., elemental tritium (HT), or as tritium water vapour (HTO). All possible migration paths, from the tritium leak to the atmosphere up to its assimilation by the exposed population or maintenance personnel, are calculated for both forms. Based on the data regarding source terms for atmospheric release obtained in ITER studies, the dispersion of elemental tritium (HT) is much higher (by one order of magnitude in some cases) than that of tritium water vapour (HTO). The analysis and assessment of the chronic dose is essential

The scenario models to be considered are: standard operational conditions, unusual events, and cases with accidental tritium release. In all cases, the concentration of HT or HTO (or both) is monitored. In the case of standard operation, NORMTRI was used. This code is based in the ISOLA V dispersion model for events with a long duration, having constant emission rates for the duration of the observation. It evaluates each dispersion process, given a certain climatologic scenario, while taking the probability for that scenario to occur into account. For the accident scenarios, the UFOTRI code, based on the MUSEMET dispersion model, will be used in order to evaluate all the atmospheric parameters, based on experimental databases, on an hourly basis.

For a complete study of the diffusion, the removal and the absorption of tritium by people, two phases are considered, simultaneously in some cases:

- Primary phase: This phase starts at the time of the atmospheric release, and concludes when the tritium is deposited in the environment (soil surface, animals or plants). Some boundary conditions have to be defined for this phase. The statistical assessment considers 4 parameters: wind speed and direction, precipitation, and stability. In turn, these 4 parameters are subdivided into several classes (for example, the wind direction is classified in terms of 10% sectors and 30% amplitude intervals over 36 or 12 sectors). Taking into account the 6 stability classes, 7 wind speed ranges are defined, as well as 4 groups of precipitation intervals, considering all the boundary conditions. The geometry is defined so that the coordinate origin is the point of release. Then, the dispersion of the cloud is analyzed, given the described parameters, and the effects of the height of the tritium release point, the ground roughness and the duration of the emission are calculated. In order to understand the importance of these factors, every event is analyzed deterministically and compared with actual probabilistic data, measured hourly, and combined with

meteorological data to provide a global study that simulates the complete dynamics of the transport and diffusion of tritium into the environment.

- Secondary phase: When the plume drops to the ground, the secondary phase is initiated. This phase starts immediately after the start of the primary phase or, in some cases, in parallel. The tritium flux into each sector of the mesh depends on the air-soil exchange rate. To estimate the tritium concentration on each point of the mesh, one must again consider all the actual meteorological parameters (solar irradiation intensity, humidity, ground roughness, etc.), as previously established in the early and subsequent phase of the release.

Tritium deposited on the surface, the vegetation, or in water can return to the atmosphere by transpiration or evaporation. Such tritium mobilization mechanisms are called re-emission processes. These phenomena affect both chemical forms of tritium, although the mechanism is different: HT from the primary plume returns to the atmosphere as tritiated water, whereas HTO may evaporate or transpire directly, without any type of conversion. The total amount of re-emission depends strongly on HT oxidation due to bacterial action in the first 5 cm of the subsoil. The re-emission increases the tritium level in the air. Thus, the re-emission must be added to the inhalation and skin absorption doses that originate directly from the primary plume. HT levels will be reduced in favour of an HTO rise. Nevertheless, the origin of this tritium increase is not caused by the primary tritium, but by the conversion of HT into HTO. The concentration loss of the initially deposited tritium is represented by an impoverishment rate that translates into a transfer rate of the surface tritium into other subsoil levels or to other elements such as roots or tubers, which will be analyzed later. These processes are strongly dependent on the environment of the deposition site, the floor and/or the vegetation, including parameters such as: floor type, porosity, Darcy laws, photosynthetic activity, humidity and solar intensity. Tritium does not remain on the surface, but it evaporates or penetrates into deeper zones, ending up in the groundwater layer. Once the tritium is deposited on the surface, tritium oxide competes with free surface water to interchange hydrogen. The tritium concentration count is made in layers of 15 cm, down to the usual depth of plant roots. Normal and tritiated water may rise due to capillary forces and due to matrix potential differences, but the speed of ascent is smaller as the potential differences decrease. Roots can absorb water until a limit is reached (the shrivelling point). At this point, water absorption by the root stops. The mentioned transport of water is strongly dependent on the structure of the floor, and in particular its porosity.

Once the tritium has penetrated and has been incorporated, the internal irradiation source is continuous, and the local dose rates increase until the tritium is eliminated from the body by sweating, excretion, or exhalation. Any remaining activity due to tritium in the body is difficult to quantify, because all process involved, the incorporation of tritium in the body, its retention and its cellular incorporation, are very complex. All the soft tissues of the human body are sensible to the radiation from tritium disintegration. In the framework of radiological protection studies, tritium dosimetry is considered to provide an all body dose, because the soft tissues make up 90% of the body weight. Furthermore, one has to consider the chemical properties of tritium, which allow it to substitute internal hydrogen easily in a large number of molecules, not only in somatic cells, but also in the genetic material. Both chemical forms of tritium, HT and HTO, can be incorporated into the respiratory tract, either by direct inhalation from the plume or by absorption through the skin. The conversion of tritium into OBT (*Organically Bound Tritium*) establishes the dosimetry of the ingestion dose calculations. These

calculations start when the early phase, involving deposition, oxidation and re-emission, is past. Because of this, the oxidised form of tritium is used for the internal dose count, whether the emission is HT or HTO.

10.3.9. Radiation damage

Material radiation damage could be studied in two ways:

- Experimentally, by analyzing the results of experiments that provide information about radiation damage of the microstructure and the mechanical material properties, or

- Theoretically, in terms of a computer simulation.

Computer simulation studies are ever more important in all fields of science due to the ever-increasing computing power available. And materials science is not an exception.

Currently, simulation methods that have a large impact on the materials are those based on an atomistic point of view. Here, the idea is obtain knowledge about the macroscopic material properties from data obtained at the atomic level. This is also the methodology currently used to develop models for the study of materials under fusion conditions. This methodology is called Multiscale Simulation.

Multiscale Simulations cover everything from 'ab initio' calculations, based on Quantum Mechanical models, through molecular dynamics, defect diffusion and dislocation dynamics, to finite element models that allow the calculation of macroscopic material properties.

10.3.9.1. The physics involved

The starting point of Multiscale Simulations is quantum mechanical calculations based on *Density Functional Theory* (DFT). Input parameters for the method on the next space-time scale level are generated from the results obtained at this level. The precision of the results at the macroscopic level depends strongly on the precision of the parameters on all lower levels, and ultimately on correct quantum mechanical data. Basically, electrons are responsible for the bonding between the atoms forming the molecules, of which the materials are composed. The nature of the electronic states determines the properties and the response of the material in extreme conditions. Nevertheless, this type of calculations is very expensive, and can at present only be performed for small molecules (consisting of a few hundreds of atoms). Results from this methodology are used to estimate interatomic potentials. The interatomic potentials are required at the next space-time scale level, Molecular Dynamics.

The DFT calculations provide fundamental properties such as the total energy. Knowing the energy exchange at the atomic positions, one can obtain information about the equilibrium geometry, the activation energy of atomic diffusivity, and the stability of the

various types of defects or dislocation structures. The forces and stress tensors can also be obtained, thus facilitating Molecular Dynamics Simulations.

A commonly used code for performing such calculations is SIESTA (*Spanish Initiative for Electronic Simulations with Thousands of Atoms*).

SIESTA is both a method and an implementation in terms of a computer program, oriented towards electronic structure calculations and *ab initio* molecular dynamics simulations of molecules and solids. Its main characteristics are as follows:

- It uses the standard Kohn-Sham self-consistent density functional method, in the *Local Density Approximation* (LDA-LSD) or *Generalized Gradient Approximation* (GGA).
- It uses atomic orbitals as a basis set, allowing unlimited multiple-zeta and angular momenta, polarization and off-site orbitals.
- It projects the electron wave function and density onto a real-space grid in order to calculate the Hartree and Exchange-correlation potentials and their matrix elements.
- It allows using localized linear combinations of the occupied orbitals, so that the computer time and memory requirements scale linearly with the number of atoms.
- It is written in Fortran 90 and memory is allocated dynamically.
- It may be compiled for serial or parallel execution.

This program provides:

- Total and partial energies.
- Atomic forces.
- Stress tensors.
- Electric dipole momenta.
- Atomic, orbital and bond populations (*Mulliken*).
- Electron densities.
- Relaxed geometry, fixed or variable cell.
- Spin polarized calculations.
- Band structure.

- K-sampling of the *Brillouin zone*.

Computational needs: the goal is to make ab initio calculations for thousands of atoms, instead of the hundreds that are typical of present-day calculations, in order to study the defects by irradiation on a scale similar to the experimental samples.

With this type of methods, typical calculations require between 10.000 and 100.000 computer hours on a normal processor.

Regarding communication, scaling behaviour with the number of processors, memory requirements, and total computing time, a typical calculation with the SIESTA code shows the following:

i) Molecular Dynamics

Molecular Dynamics (MD) is a simulation technique used in the field of Physics and Chemistry of the Solid State. In this technique, atoms and molecules can interact for a period of time. In general, molecular systems are complex and are made up of a large number of particles. This makes it impossible to write their properties in an analytical form. To circumvent this problem, MD uses numerical methods. The technique forms is at a crossroads between experiment and theory, and it may be viewed as a computer experiment.

Molecular Dynamics is an interdisciplinary field. The laws and the theory derive from Mathematics, Physics and Chemistry. It makes use of algorithms from Computational Science and Information Theory. Molecules and materials are not described as rigid entities, but rather, as evolving bodies. Its original application was in the field of theoretical physics, but currently it is used mostly in biophysics and material science. Its fields of application vary from catalytic surfaces to biological systems.

This technique shows that a link exists between computational cost and the reliability of the results, as it uses Newton's equations, which are less expensive than quantum mechanical equations. For this reason, some properties cannot be studied with this methodology, such as the breaking and formation of bonds, since excited states or reactivity cannot be handled.

Hybrid methods exist, called QM/MM *(Quantum Mechanics/Molecular Mechanics)* models. These models treat reaction centre using quantum mechanics, and the remainder using classical theory. With these methods, the challenge lies in defining the precise interaction between the two descriptions.

Microcanonical Ensemble (NVE). The simplest model of molecular dynamics is obtained using the microcanonical ensemble description. In such an ensemble, the system is considered isolated: the volume (V) does not change and it does not exchange mass (M) or energy (E) with the environment. In a system consisting of N particles with coordinates X and velocities V, one derives first order differential equations. The potential energy function U(X) describes the attraction and repulsion between the atoms due to the chemical bonds, electrostatic interactions, Van der Waals forces, etc. U(X) is also known as the force field and it is a function of the particle coordinates X. Usually it is derived from quantum chemical calculations and/or spectroscopic experiments. Nevertheless, the force field has a functional form that is typical of

classical mechanics. The particle trajectory is discrete in the time co-ordinate. Usually, a small time step (e.g., 1 fs) is chosen in order to avoid numerical errors due to the discretization. The position X and the velocity V are integrated using a simplistic integration method, such as the Verlet method, for each time step size. Given the initial positions (e.g. the X ray structure of a protein) and the initial velocities (e.g. random and Gaussian) one may calculate all the positions and velocities in the future.

Other ensembles (NVT, NPT). Other methods exist, with different characteristics for similar systems, such as systems with a constant temperature or a constant pressure. These methods greatly enhance the utility of MD for the systems under study.

The Software codes that are most commonly used for computational Molecular Dynamics calculations are the following:

- *LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) and MDCASK* are the most commonly used computational codes in material science. LAMMPS was developed at Sandia National Laboratories, a US Department of Energy laboratory, and MDCASK was developed at Lawrence Livermore National Laboratory, also a US National Energy Supercomputer Centre. Both are parallel codes, and capable of using multiple processors during a calculation, thus increasing the size and timescale of the systems that can be studied. The scalability, i.e., the efficiency of the parallelization, is almost linear. Therefore, by increasing the number of processors, calculations can be performed for a larger number of particles interacting for more time, thus increasing ergodicity and statistics.

- *Kinetic Monte Carlo.* Kinetic Monte Carlo (KMC) is a Monte Carlo method intended to simulate the time evolution of some specific naturally occurring processes. Typically, these are processes that occur at a given known rate. It is important to understand that these rates are inputs to the KMC algorithm, and the method itself cannot predict them.

  The KMC method is essentially the same as the dynamic Monte Carlo method and the Gillespie algorithm. The main difference appears to be in the terminology and the applications: KMC is used mainly in physics, while the 'dynamic' method is mostly used in chemistry.

  By way of example, the KMC algorithm for simulating the time evolution of a system in which some processes occur at known rates r can be written as follows:

  i. Set the time t = 0.
  ii. Form a list of all possible rates in the system r_i
  iii. Calculate the cumulative function for i = 1, etc. N where N is the total number of transitions.
  iv. Obtain a uniform random number u' [0, 1]
  v. Determine which events will occur by finding the i for which $R_{i-1} < u'R \leq R_i$.
  vi. Carry out the event i.

vii. Recalculate all rates r_i which may have changed due to the transition. If appropriate, remove or add new transitions i. Update N and the list of events accordingly.

viii. Obtain a new uniform random number *u* [0, 1].

ix. Update the time with t = t + Δ*t* where Δ*t=-log u/R*.

x. Return to step 2.

In different sources, this algorithm is known variously as the residence-time algorithm, the n-fold way, the Bortz-Kalos-Liebowitz (BKL) algorithm, or just the kinetic Monte Carlo (KMC) algorithm.

KMC has been used in simulations of, e.g., the following physical systems: surface diffusion, surface growth, vacancy diffusion in alloys (this was its original use in (Young 1966)), defect mobility and clustering in solids irradiated by ions or neutrons.

To give an idea what these 'objects' and 'events' may be in practice, here is one concrete and simple example, corresponding to example 2 above.

Consider a system in which individual atoms are deposited on a surface, one at a time (typical of physical vapour deposition), and which can also migrate across the surface with some known jump rate w. In this case, the 'objects' of the KMC algorithm are simply the individual atoms.

If two migrating atoms arrive at adjacent locations, they become immobile. The flux of incoming atoms determines a rate $r_{deposit}$, and the system can be simulated with KMC by considering all deposited mobile atoms which have not (yet) met a neighbour and become immobile. Thus, the following events are possible at each KMC time step:

- A new atom arrives with a rate given by $r_{deposit}$
- An atom that has already been deposited makes a jump with rate w.

When an event has been selected and the KMC algorithm has evaluated it, one needs to check whether the new or migrated atoms have become immediately adjacent to some other atom. If this is the case, the adjacent atom(s) need to be removed from the list of mobile atoms, and their jump events removed from the list of possible events.

Naturally, when applying KMC to problems in physics and chemistry, one has to consider first whether the real system matches the assumptions underlying KMC to a sufficient degree. Real processes do not necessarily have well-defined rates, the transition processes may be correlated, the jumps of atoms or particles may not occur in random directions, and so on. Also, when simulating widely disparate time scales, one needs to consider whether different processes may occur on longer time scales. If any of these considerations apply, the time scales and the system evolution predicted by KMC may be biased, or even completely wrong.

KMC methods can be subdivided according to the type of motion or the nature of the reactions. The following, incomplete, classification is often used:

- Lattice KMC (LKMC) methods refer to KMC on an atomic lattice. Often, this variety is also called atomistic KMC, (AKMC). A typical example is the simulation of vacancy diffusion in alloys, in which a vacancy is allowed to jump around the lattice with rates that depend on the local elemental composition. A code of this type that is commonly used is LAKIMOCA, developed by EDF in France.
- Object KMC (OKMC) methods refer to KMC applied to defects or impurities, jumping in either random or lattice-specific directions. Only the positions of the jumping objects are included in the simulation, not those of the 'background' lattice atoms. The basic KMC step is one object jump. A code using this method is BIGMAC, developed at LLNL, USA.
- Event KMC (EKMC) or First-passage KMC (FPKMC) refers to a variety of OKMC in which the next reaction between objects (e.g., the clustering of two impurities, or vacancy-interstitial annihilation) is chosen by the KMC algorithm, taking into account the positions of the objects, and this event is then immediately carried out (Dalla Torre 2005, Oppelstrup 2006). The code most commonly used is JERK, developed at CEA, France.
- Parallel KMC (PKMC) is a modification of the OKMC algorithm that allows a parallel implementation. Due to this, the study of larger systems, during a longer period of time, becomes possible. The algorithm and its implementation have been developed recently by the UPM (Spain) in collaboration with LLNL, USA.

However, in practice, Monte Carlo simulations are limited to small volumes (cubes of up to 1 μm, depending on the conditions) and become computationally expensive when the irradiation dose is high and/or when time scales of the order of nuclear reactor lifetime are explored.

This limitation can be overcome by using rate theory (RT) as an alternative. In this approach, based on the mean-field approximation, the diffusion of defects is modelled by means of a set of diffusion-reaction rate equations, while the nucleation and/or the growth of clusters is described by the master equation. In this model, the evolution of the medium concentration of an impurity or the evolution of a cluster of a given size is governed by a continuity equation. The system is represented by a set of connected partial differential equations (from hundreds to thousands of equations). Rates, such as the diffusion coefficients or the dissociation frequencies, are calculated from the KMC input data, so these two methods are based on the same parameters.

The RT approach is attractive due to its reduced computational requirements, thus allowing the exploration of defect evolution over large time scales and distances, close to the experimental values. However, one of the basic assumptions in the mean-field approximation is that defect production is uniform in time and space, and set at some appropriate value. In other words, rate theory does not consider the position of each of the defects but it calculates the medium concentration of each type of defect. When complex mechanisms are considered, results obtained by RT

models can deviate from those obtained by KMC. For example, RT cannot deal with the recombination of correlated I-V defects generated by irradiation.

KMC and RT are complementary methods and can be used in a multiscale simulation strategy.

The RT code PROMIS 1.5 has been developed by S. Selberherr and P. Pichler at the Technological University of Vienna. It allows solving general diffusion equations in 1D or 2D under general environmental conditions. Generation-recombination terms, boundary conditions and a diffusion flux that is directed or induced by an electric field can be easily implemented if necessary. Input parameters are the same as those in KMC.

With KMC, the position of each defect is stored. Therefore, the computational requirements increase linearly with the number of defects (for example, in the case of a high irradiation dose). A typical problem might require a few days of computation, or several thousands of hours. Therefore, KMC calculations require a significant computational effort.

RT imposes very little computational requirements. A typical experiment involving He desorption, involving thousands of partial differential equations, would require only a few minutes of calculation on a typical Pentium processor. On the other hand, obtaining free parameters from experimental data may require hundreds or thousands of simulations. In any case, RT may require only a moderate computational effort, in given cases.

ii) Dislocation Dynamics

In distorted materials, crystal plasticity is determined by the collective behaviour of major dislocations. Although laws could be written down for the continuum that describe the macroscopic behaviour of the material under a variety of loading conditions, based on efficient density dislocations, the movement of dislocations and their mutual interactions are heterogeneous phenomena that show an intrinsic dependence on the underlying microstructure. The details of these interactions are usually quite important but are not captured by continuum models that are based on the mean dislocation density. Therefore, atomic methods are commonly used to study the interaction mechanisms of isolated dislocations. However, these methods only describe a limited range of space-time scales, and therefore incorrect results are obtained when one attempts to apply it to the dislocation stress field in the long range, or to describe the statistical nature of the crystal plasticity.

An alternative method is provided by Dislocation Dynamics (DD), which is a direct approach that tries to simulate the collective behaviour of major dislocations on the mesoscale. It does this by breaking down the random curvature dislocation lines in rectilinear segments[170]. However, the number of segments, N, could be large for meaningful simulations, and the long range force calculation requires an effort $O \sim N^2$. Because of this, the problem can be computationally expensive for large systems. For a comprehensive revision of this topic and

[170] Kubin et al., 1992; Devincre y Kubin, 1997; Kubin et al., 1998; Zbib et al., 1998; Schwarz, 1999; Ghoniem y Sol, 1999; Zbib et al., 2000; Bulatov et al., 2001; Cai et al., 2004.

DD in general, please refer to Zbib and Diaz de la Rubia (2002) and the bibliography cited in that reference.

The use of DD for modelling some aspects of crystal plasticity in 3D in fcc metals was established at the end of the 80's in the pioneering work of Kubin et al.[171] and Ghoniem et al. [172]. Nevertheless, studies involving complex geometries and large dislocation densities have not been attempted until just a few years ago. [173].

Dislocations are described as a set of nodes, connected to each other by rectilinear segments. The node positions and their connections are called the fundamental degrees of freedom. If a node is connected with n other nodes, it is called a node with a connectivity n. In general, the computational cycle is as follows:

i. Calculate the driving forces ~ fi for each of the nodes.
ii. Calculate the velocity ~vi of each node based on ~ fi and the local dislocation nature.
iii. Set the time step _t.
iv. Evolve all the dislocation nodes in time to t + _t, handling topological changes during [t, t + _t].
v. t: = t + _t. Return to a i.

The two codes that are primarily used by material scientists are ParaDis and Micro3D. Both codes are massively parallel. This increases the maximum number of dislocation segments that can be studied considerably.

In summary, the main experimental features of the Computer Simulation Facility of *TechnoFusión* are:

- **Simulation**
  - Basic research
  - The area is essential in a prestigious centre
  - National experts of known prestige are present, and more can be incorporated
  - The collaboration with other university groups is guaranteed
  - Computational platforms are available (Europe and Spain)
  - Proper platforms (for development, independence)
  - Additional value (a proper centre and external users)

- **Acquisition and Control**
  - An experimental centre requires a centralized computing service for the acquisition and control of data
  - Access, coherence, scalability, security, …
  - The possibility of proper developments (I+D+i, R&D)
  - Collaborations with other groups and industries
  - Solve users' problems and facilitate the operation of the Centre.

[171] Lepinoux y Kubin, 1987; Kubin et al., 1992
[172] Ghoniem y Amodeo, 1988; Amodeo y Ghoniem, 1991.
[173] Verdier et al., 1998; Shenoy et al., 2000; Espinilla et al., 2001; Dupuy y Fivel, 2002; Madec et al., 2002; Kubin et al., 2003; Depres et al., 2003; Shehadeh et al., 2005; Devincre et al., 2006.

- **Analysis and Visualization**
  - A new scientific paradigm
  - Data acquisition and generation on a scale not seen before
  - Analysis processes less developed
  - Extraction of all the available information
  - Development of proper techniques
  - Collaboration with other groups (biomedicine, …)
  - Feedback to the national industry

- **Media**
  - Openings for network and office personnel
  - The acquisition, management and support of computer supplies (hardware and software)
  - Consistent centralised management
  - Controlled private networks, acquisition and storage
  - Networks for the connection to other centres and Internet
  - Security

- **Human Resources**
  - Scientists in the field of materials science, plasma physics, nuclear physics, fluid dynamics; robotics and electronic engineers (simulations, …), and computational science scientists (algorithms, …)
  - Technicians
  - Programmers, analysts, operators
  - Personnel for design, essays and production (laboratories, …)
  - Administrative personnel (management, purchases, training, …)
  - Contacts and collaborations are essential

- **Computer Resources**
  - Generics
  - Internal and external (secure) networks
  - Administrative office positions
  - Specifics
  - Storage (secure and massive)
  - Processing (access, analysis and visualization)
  - Computing (development and production)
  - New developments (control, acquisition, real time, …)

Table 10.1 shows the status of art in the different simulation models described above, as well as the experience, development, validation and final use carried out by the people of the CS Facility of *TechnoFusión*.

Table 10.1. State of the art in model simulation by thematic areas and simulation models (E) Experience, (D) Development, (V) Validation, (U) final Use.

Area Code	Level of knowledge	Area Code	Level of knowledge
Nuclear data		**TH System**	
Activation Library EAF2003/05/07	E	RELAP INEL-NRC.USA	E, D, V, U
Transport Libraries JEFF31 ENDF/B-VII JENDL-HE FENDL HENDL	E	**Sensitivity and uncertainties**	
		SUSD3D Uncertainty code package. NEA/Kodeli I.	E, D, V, U
		Containment	
Nuclear Data Processing Codes		CONTAIN Sandia/NRC.USA. Termohidráulic of containment	E, D, V, U
NJOY LANL.USA/JEFF.NEA Libraries of ENDF/JEFF	E, D, V, U	**Severe Accidents**	
PREPRO2000 LLNL/D.E. Cullen	E, D, V, U	MELCOR Sandia/NRC.USA. integral code of serious accidents	E, D, V, U
Nuclear Physics Codes			
TALYS Simulation of nuclear reactions NRG/A. Koning	E, D, V, U	MAAP/SCDAP NRC.USA. Severe Accident Phenomena and Plant Evaluations – FAI	E, D, V, U
EMPIRE-II Nuclear Reaction Model Code IAEA	E, D , V, U	**Radiation Damage**	
		PERFECT/GETMAT EU-FP6/FP7	E, D, V, U
Transport Code: Monte Carlo			
TRIPOLI EU-NURESIM (CEA.fr)	E, D, V, U	MDCASK (Classic Molecular Dynamic)	E, D, V, U
MCNP LANL.USA	E, D, V, U	BIGMAC (Deffects Diffusion – MonteCarlo)	E, D, V, U
PHITS Particle & Heavy-Ion Transport (KEK.jp)	E, D, V, U	SIESTA ("ab-initio")	E, D, V, U
		LAMMPS (Classic Molecular Dynamic)	E, D, V, U
FLUKA/GEANT CERN	E, D, V, U	DD3D (Dislocation Dynamic)	E, D, V, U
		TBSiC (DM Tight Binding for SiC)	E, D, V, U
PENELOPE NEA/Univ. Barcelona.es	E, D, V, U	**Evaluation, location, ambient dose, tritium**	
Transport Code: SN		GASPAR/LADTAP/XOQDOQ NRC.USA (Fluents Dose)	E, D, V, U
TORT-DORT neutron & gamma SN Transport ORNL	E, D, V, U	MACCS2 RSICC.USA radiological and economic consequences of accidents	E, D, V, U
ATILA neutron & gamma			
TWODANT/THREEDANT			
Geometric Interface		PC-CREAM Metodology of European Comission Dose of Efluents	E, D, V, U
MCAM	E, D, V, U		
McCAD			
GEOMIT		COSYMA FZK y NRPB, European Comission. Radiologic and economic consequences of the accidents	E, D, V, U
DAGMC			
SNAM			
Graphic Interface			
VisualBUS		**Analysis of statistical probability**	
MORITZ	E, D, V, U	SHAPHYRE 6.0 INEL for the NRC, USA	E, D, V, U
SABRINA			
Isotopic and Activation Inventory			
ORIGEN/SCALE ORNL+LANL.USA	E, D, V, U		
ACAB UNED.es	E, D, V, U		
FISPACT UKAEA	E, D, V, U		
MONTEBURNS MCNP+ORIGEN/CINDER LANL.USA	E, D, V, U		
TH CFD			
ANSYS-CFX Commercial (ANSYS.USA)	E, D, V, U		
FLUENT *Commercial (ANSYS.USA)*	*E, D, V, U*		

10.4. Layout, supplies and safety requirements

(I) Physical spaces and facilities

Since it is envisioned that use will be made of large national computer facilities, the CS Facility does not need to have an extensive infrastructure; specifically, the following physical space would be needed:

- One 30 m^2 room to accommodate the analysis equipment and acquisitions.
- One 30 m^2 room for the instruments and auxiliary machines.
- One 20 m^2 warehouse.
- 100 m^2 for personnel offices and services.

(II) Safety

The CS Facility should comply with the Law of Professional Risks (BOE nº 269, 10/11/1995 (R.D. 31/1995)).

Nowadays, computer simulations may require long periods of time for processing and operation, so that power cuts or power surges in the local electrical network should be avoided as much as possible. Therefore, *Uninterruptible Power Supply* (UPS) systems are needed. These systems can provide current during a power interruption for at least some hours. In this way, the acquisition and processing systems and the general data storage servers can be protected.