2nd part: Challenges and developments on advanced computational tools for ITER neutronics

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Outline

- **Introduction to ITER neutronics analysis**
- **Acceleration of Monte Carlo ransport calculations**
- **Geometry Modelling in Monte Carlo Transport Calculations**
- **Coupling radiation transport-activation schemes and shutdown dose rate calculations**
- **Summary and last comments.**

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Computational Neutronics simulations in ITER for faithful calculations

- **Neutron (and photon) transport simulations**
- **Coupled activation and radiation transport calculations**
- Determine the distribution of the neutron (prompt and decay photons) population and the physical observables related to the behavior of the population (nuclear responses)
- Quantities needed: integrated/component; and differential/3-D mesh **(high resolution)**
- **Geometry:** Large , **complex,** with significant heterogeneity and streaming paths
- **Requirements:** **Suitable computational approaches and tools**; high-quality nuclear cross sections data; and accurate-enough simulation models of the real geometry.
- Far of this ten years ago. Now in an acceptable situation. ¿ what have been the challenges and developments on advanced computational tools? How we do ITER neutronics today.

Selection of a suitable method for simulation of neutron transport in ITER

- **Requirements**
  - handle a complex geometry with high fidelity and sufficient detail
  - employ nuclear cross-section data without severe approximations
  - Can be coupled with nuclide inventory codes for **coupled radiation transport and activation calculations**
- ***In principle, fulfilled by Monte Carlo (MC) particle transport technique***
  - full 3D geometry without the need for real approximations. **¿Are easy to create?**
  - continuous energy nuclear interaction cross-sections can be used
- The accuracy of the MC only affected by the statistical uncertainty of the calculation
  - no numerical approximation in the MC calculation, no transport equation need to be solved
- Inherent drawback: For acceptable statistical uncertainty a big number of followed particles is likely required (**unacceptably slow** for practical applications)
- Major changes in the application of MC codes for ITER : **acceleration; geometry; coupling transport-activation.**

Acceleration of MC transport calculations

- Major changes in the application of MC codes for ITER : **acceleration;** ~~**geometry; coupling transport-activation**~~.

MC METHOD and application to neutron and photon transport: Basics ideas

- **MC Method (main elements)** : stochastic model; and a certain random variable (estimator) whose expected value is equivalent to the value of a physical quantity to be determined.
  - estimated by the average of several/many independent samples of the variable
- **MC Transport simulation: Simulate de transport (life) of individual neutron** histories from birth to death (microscopic level); and compute the value/score of the **estimator** (tally) of the physical quantity of interest.
- Simulating enough neutron histories makes it possible to quantify the macroscopic physical quantities. (transport on the macroscopic level)
- If MC with a Infinite number of histories
  - **Average** of the scores be true **value** (true mean) **of the physical quantity.**
- A real MC simulation: Number of histories finite, **N**.
  - **Sample mean** as an estimate of the true mean
  - **Error** (standard deviation), how far the estimated mean is likely to be from the true mean.
  - Intended to be a small enough value. It is proportional to $1/\sqrt{N}$
- The most straightforward Monte Carlo calculational method: *analogue MC* simulation:
  - **natural probabilities of the physical transport process**
  - very limited range of application

Acceleration of MC transport calculations

- ***Non-analogue MC* approach/variance reduction**: well-founded modified probabilities and corresponding unbiased estimator in such a way that can lead to the same result in the estimates of the quantities than those using the natural probabilities.
- Traditionally, VR techniques aimed to an individual localized phase-space region
- Modern VR techniques (over the last 10 years), called global variance reduction (GVR) enables:
  - determine a quantity (e.g., flux, dose rate, etc) in multiple localized regions, or even distributions of a quantity **with uniformly low statistical uncertainty throughout the entire/global problem space**.
- GVR methods relays on using information previously obtained, as fast and effortlessly as possible, on the distribution of the neutron fluxes. Two approaches:
  - Stochastic. MC/MC methods
  - Deterministic. Hybrid Monte Carlo/Deterministic methods
- **Parallel computation**: MC method is inherently parallel (particles are simulated independently).
- An **efficient combination of parallel computing** and the application of strong **GVR techniques** have been developed,
  - avoiding a significant reduction in the efficiency of parallel computation (long history effect)
  - **Dramatically increased the performance of modern MC codes**.
- Optimize GVR techniques is an active field of research and making them more user friendly.

Neutron and photon transport at UNED

- **The MCNP (LANL) transport code** is our basic computational tool**.**
- Relevant extensions of the native MCNP (V5 and 6) developed to satisfy ITER neutronics needs. Resulting in the **MCUNED code.**
- Transport simulation in high-detail geometry models is done by:
  - massive-parallel MC radiation transport
  - With mesh-based VR reduction techniques and source biasing; and obtention of GVR parameters via MC.
- **Cell under voxel** and mesh-based results for high resolution distributions of neutrons flux and nuclear responses

Geometry Modelling in MC Transport Calculations

- Major changes in the application of MC codes for ITER : ~~**acceleration;**~~ **geometry**~~**; coupling transport-activation**~~**.**

Some Modern Geometry Modelling capabilities in MC Transport Calculations

- MC method: potential to be applied on arbitrary 3-D geometric configurations
- In practice, MC codes have provided a limited geometry modelling capability
  - only an approximation of the realistic geometry could be made available
- Main drawback: the user is required to define the geometry manually. Strong impacts
    - Constructive Solid Geometry (CSG): defining geometrical regions from all the first- and second-degree surfaces of analytical geometry and elliptical tori and then of combining them with Boolean operators
- A new way of producing detailed geometry desperately needed (10 years ago)
- Ability to use CAD models in MC radiation transport. Main types of approach
  - Translating the CAD geometric representation (in Boundary REPresentation, BREP) into the representation (CSG) of the MC code. **Translational approach**
  - Changing the internal geometric representation used within the MC transport code.
    - **Direct approach**. Direct tracking of MC particles on the CAD geometry.
    - **unstructured Mesh** (UM) geometry descriptions
- The most matured approach for ITER is the translational approach

Workflow to convert CAD models into MC-CSG geometry and built complex transport models

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- Inputs for ITER neutronics analysis
  - Neutronic ITER reference model (C-lite, E-lite). It is built in CGS-MCNP format
  - CAD engineering model of the component.
- Actions
  - Creation of the Neutronic MC Model: simplification and conversion to MC
  - Integration with ITER reference model (well established procedure):
- Model creation: geometry conversion from CAD to MC
  - Preparation phase: Developed on CAD platform (CATIA, SpaceClaim, ...)
    - CAD clean-geometry model: Fixing of geometry errors (gaps, overlaps, etc.,).
    - CAD-Neutronic model. Removal of neutronically unnecessary details
    - CAD Netronic model for conversion to CSG-MCNP
      - Replacement of surfaces described by spline functions
      - If required, pre-decomposition of rare complex models
  - **Conversion of prepared CAD geometry model to MC geometry**
    - Decomposition in primitive solids + translation + addition of void spaces (automated with a suitable geometry conversion tool)

Geometry at UNED: Simulation steps related to the geometry

- **Perform geometry conversion from CAD to MC geometry**
  - Preparation phase is undergone with SpaceClaim
  - **Conversion to MC/CSG geometry with MCAM (ASIPP, China)**.
    - **The home-made GEOUNED is starting to be used**
- **Perform simulation and geometry**
- Two of the many steps involved to perform simulation are closely related to the geometry management
  - reading and processing of the geometry information, and
  - simulation of random walk histories within this geometry
  - MCUNED transport module/based in MCNP: developments in both of them
- **Memory management related to the geometry**
  - Modifications to loading-, storing- and plotting native MCNP routines
  - Important effect to **save the RAM memory** used to store the geometry (79%), reduce the **loading time** (98%)
  - This has been **crucial for handling the increasingly complex geometry models** (such as E-lite)
- **Simulation of the Random walk**
  - More efficient algorithm for **the ray-firing process** of determining the next geometrical cell boundary (20% **speed up**, C-lite model). Enable **faster visualization** (easy geometry checking for lost particles)

Coupling radiation transport-activation schemes and shutdown dose rate calculations

- Major changes in the application of MC codes for ITER : ~~**acceleration**~~**;** ~~**geometry**~~; **coupling transport-activation.**

Shutdown Dose Rate Calculations (SDR)
Coupling transport-activation calculations

- Radiation after shutdown ("post irradiation") is due to decay photons emitted by radioactive nuclides. Theoretically, three computational steps are required for SDDR mapping
  - Neutron transport calculation for the spatial and energy distribution of the neutron flux spectra,
  - Activation/Nuclide inventory calculation to obtain decay photon source distribution (spatial and energy), and,
  - Decay photon transport calculation to obtain dose rates at the locations of interest.
- *Likely to be one of the most difficult problems to deal with in neutronics: neutron induced activation and decay photon transport simulation. And expensive in terms of computational effort.*
- *Two approaches implemented based on MC particle transport simulation.*

Rigorous 2-Step (“R2S”) Method

- Neutron transport and photon transport simulations are done separately, coupled by a nuclear inventory analysis code, using suitable interface scripts.
- For transport a MC code is utilized and for activation a full nuclide inventory code with a comprehensive modelling of activation, transmutations and depletion.
- In principle, it is of general application. But with some limitations on the accuracy
  - Transport by MC enable the geometry to be represented continuously, but as for the activation step a discrete geometry representation (mesh-based description of materials) is required
- The implementation of this approach has followed different improved methods:
  - **cell-based** method ; super-imposed **mesh-based** method
    - limitations due to the spatial gradients of the neutron flux and the decay gamma source
  - **cell-under-voxel** method:
  - **unstructured mesh**
    - Overcoming the limitations

R2S at UNED. R2SUNED code system

- **Transport: MCUNED transport code (mode R2S).**
- Options for the super-imposed mesh-based method and **Cell-under-Voxel (CuV) method.**
- The CuV technique is original from UNED: differentiation of materials and fluxes within the voxels of a structured mesh
  - Included within the unified European R2S code system, called cR2S (“common R2S”), under development by CCFE, KIT and UNED
  - Voxels containing different materials, CuV generate a different tally for each material corresponding to the real flux, not to the voxel averaged-flux.
- **Activation step**: **performed by the ACAB/UNED** code and can follow two strategies:
  - multi-group neutron fluxes and multi-group neutron activation cross-sections
  - **Reactions rates calculated in the MC transport calculation (pre-analisis step needed**)
  - Additionally, enabling the possibility for **energy-wise photon emission density**
- **Propagation of uncertainties** from the MC neutron transport calculation to the SDR uncertainty

Direct-one-Step (D1S) Method

- **Performs the neutron and decay-photon transport simultaneously in the MC simulation**.
  - **Couple the emission of decay gamma rays to the neutron cross section producing the radioactive isotope**
    - Replacement of prompt photons by decay gammas in the MC transport calculation
- It is the most accurate (no discretization needed for any variable) when **linear dependence between the activity** of the radioisotope of interest and its **production rate**:
  - radioisotopes are produced in simple activation chains/pathways
    - a direct path (one reaction). O no direct pathways but consisting of only one neutron reaction
  - Negligible burn up of parents and radioactive isotopes.
- **Special purpose D1S activation data files**
  - Replacement of transport with activation cross-section data
  - Replacement of prompt photon production data (yields & spectra) by decay gamma data
- No need of activation calculation for decay gamma sources. **Adjustment factors requires**
  - Ratio of the actual activity over the production rate
  - *Depending on radio-nuclide and irradiation-cooling history.* Easily calculated
- **Activation pre-analysis** to know the most *important* radio-nuclides and activation cross sections

D1S at UNED. And quality assurance R2S&D1SUNED

- **D1SUNED system is the refence code in ITER for shutdown dose rate calculations**
- **Software of reference for generation of D1S dedicated activation/transport libraries.**
- **MCUNED/D1S-mod with pioneering capabilities on**:
- **Generation of decay gamma source (DGS) and flux&NRs distributions.**
- **Mapping the contribution of each DGS location/voxel to a specific tally (dose rate).**
- Contribution of the different the activated components to the dose rate (filtering)
- Contribution of the different daughter radionuclides to the dose rate; and contributions due to the presence of the different parents (filtering).
- **Different irradiation-cooling scenarios for different components in the same simulation**
- **Assign different geometric models to irradiation and shutdown phases**.
- **Comprehensive activation pre-analysis with ACAB/UNED code**
- **Quality assurance MCUNED/R2S &D1S**: Verifyed, benchmarked and validated for FNG (Frascati Neutron Generator) 14 MeV neutron irradiation experiment and **JET dose rate measurements (D-D, D-T).**

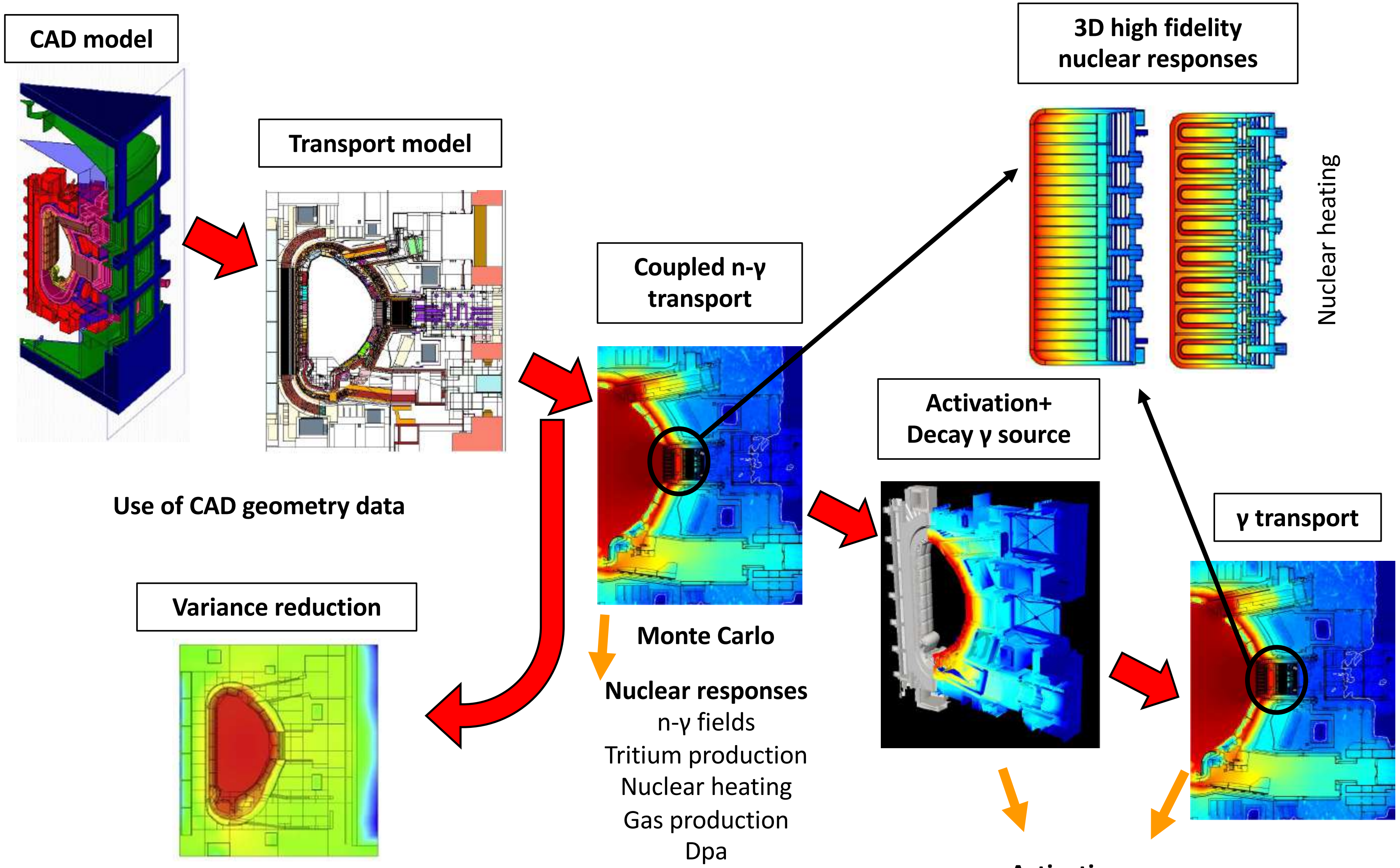
Source routines developed at UNED

- Custom source routines are needed.
- Reading external data describing the source and specify the sampling of source histories
- Essential to provide novel capabilities
  - **R2S & D1SUNED Decay gamma source**
  - Generation of intermediate detailed surface sources (cylindrical and plane) for neutronics analysis beyond the bioshield. **SCRUNED Methodology**: adopted by ITER IO.
  - Source transferred to any arbitrary geometry/problem for SDR mapping
  - **Moving Sources for accumulated absorbed dose mapping**
  - **Modelled Source of a component contaminated with activated dust**
  - Modelled Source of activated cooling water
  - Parametric plasma source (given by ITER reference models)

Summary and last comments

- Major changes in the application of MC codes for ITER : ~~acceleration;~~ ~~geometry~~; ~~coupling transport-activation; (and sources)~~

Neutronics workflow ¿implemented with home made codes?



CAD model

Transport model

Use of CAD geometry data

Coupled n-γ transport

Monte Carlo

Nuclear responses
n-γ fields
Tritium production
Nuclear heating
Gas production
Dpa
Prompt dose

Variance reduction

Weight maps for GVR

3D high fidelity nuclear responses

Nuclear heating

Activation+ Decay γ source

γ transport

Activation responses
Nuclide inventory, decay γ field, decay heat and Shutdown dose

Summarizing and last comments

- ITER has driven an impressive advance of computational neutronics.
- Advanced methods and computational tools are developed to produced nuclear response results with high-fidelity and high-resolution on the ITER complex geometry.
  - demanding for neutronics (neutron flux for SDR) and other physics (nuclear and decay heat) involved in the engineering design of ITER systems.
  - Developments have fulfilled most of the neutronics needs of DEMO
- If choosing the two developments likely to be of the most impact: MCAM and D1SUNED
- Spanish groups (CIEMAT, UNED) can address the complete workflow for ITER neutronics analysis. Proprietary codes and software that they have developed are used for some of the tasks. Highly detailed, accurate and reliable simulations and models are offered.

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Thanks for your attention

Gracias por su atención