Influence of the ab-initio nd cross sections in the critical heavy-water benchmarks

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Abstract

The n-d elastic and breakup cross sections are computed by solving the three-body Faddeev equations for realistic and semi-realistic Nucleon-Nucleon potentials. These cross sections are inserted in the Monte Carlo simulation of the nuclear processes considered in the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP). The results obtained using these \textit{ab initio} n-d cross sections are compared with those provided by the most renown international libraries.

1 Introduction

Monte Carlo simulations of neutron transport are broadly used in many domains of applicative nuclear physics. A key ingredient in these simulations is the knowledge of the nuclear cross sections. They are determined by evaluating the existing experimental data and compiled in the widely used nuclear data libraries. This is of course the most canonical and legitimate approach. However accurate experimental data is not always available and for some particular reactions may be very costly or even impossible to attain. In such a case, the models based on nuclear data evaluation and extrapolation would lack in credibility. On the other hand, and from a scientific point of view, the most satisfying solution would be to get predictions of the desired cross sections by a reliable theory derived from the first principles (i.e. nucleon-nucleon interaction). Such idealistic approach still remains somehow utopic both due to the longstanding puzzle of the nucleon-nucleon interaction and to our inability to solve the underlying scattering problem for complex nuclear systems.

Nevertheless during the last few decades reliable theoretical tools have been developed to describe few-nucleon scattering starting from the nucleon-nucleon interaction. In particular neutron-deuteron system is well explored, enabling accurate and complete description both for the elastic and three nucleon break-up processes. Furthermore neutron-deuteron cross sections turn to be predetermined by the well controlled long range part of the nucleon-nucleon interaction. This fact makes us believe that the n-d cross sections obtained from the first principles can be successfully applied in Monte Carlo simulations as well as to enrich the evaluated nuclear data libraries.

The paper is organized as follows. We present in Section 2 the theoretical tools used to solve the three-body problem and to computed the corresponding cross sections.
The results provided by some selected nucleon-nucleon potentials are compared to the existing experimental data in Section 3. Section 4 is devoted to describe the different sets of heavy water benchmarks for which the Monte Carlo simulations will been performed. The results of the multiplication factor $K_{\text{eff}}$ obtained by Monte Carlo simulations including the ab initio cross sections are presented in section 5. Some conclusive remarks are finally drawn in Section 6.

2 Computing the nd cross sections

Our aim in this section is to describe the theoretical tools we have used to compute the \textit{ab initio} neutron scattering on a deuteron, in the non relativistic quantum mechanical framework provided by the Faddeev equations $\text{[1]}$.

2.1 Kinematical variables

We consider an incoming neutron ($m$) with laboratory kinetic energy $T_L$ and momentum $p_L = \sqrt{2T_L m}$ impinging on a deuteron considered at rest. We are interested in the energy domain of $T_L \in [0, 30]$ MeV and restrict to the non-relativistic kinematics.

In order to simplify the dynamical equations, we have considered that proton and neutron have identical mass $m_p = m_n = m$, and take $\hbar^2/2m = 41.47$ MeV fm$^2$. For the neutron energies exceeding $T_L \geq \frac{3}{2}B_d = 3.34$ MeV, where $B_d$ is the deuteron binding energy, the three particle break-up channel is open, whereas at lower energies only elastic scattering of neutron is possible.

![Figure 1: Kinematical laboratory variables in the n-d elastic scattering (left) and break-up reaction (right).](image)

The momentum conservation laws for the elastic and break-up processes in the laboratory frame are displayed in Fig. 1.

In the elastic channel the final state is determined by the momenta of the scattered neutron $\vec{p}_1$ and deuteron $\vec{p}_2$. These are a priori six unknowns, satisfying the four dynamical equations

\[
\vec{p}_L = \vec{p}_1 + \vec{p}_2, \quad \frac{p^2_L}{2m} = \frac{p^2_1}{2m} + \frac{p^2_2}{4m} \tag{1}
\]

letting two free kinematical variables.

In the break-up channel, the final state is determined by the momenta of the three outgoing particles. We will denote by $\vec{p}_1$ and $\vec{p}_2$ the neutron momenta (here considered as
distinguishable particles) and by $\vec{p}_3$ the proton one. This gives a priori nine unknowns, constrained by the conservation laws

$$\vec{p}_L = \vec{p}_1 + \vec{p}_2 + \vec{p}_3$$  \hspace{1cm} (2)

$$\frac{p_L^2}{2m} - B_d = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{p_3^2}{2m}$$  \hspace{1cm} (3)

and giving five free kinematical variables.

There exists several possible ways to choose the independent kinematical variables among the momenta $\vec{p}_i$ defining the final state. It is useful to express all of them in terms of the relative Jacobi momenta $\vec{p}$ and $\vec{q}$ defined by

$$\vec{p} = \frac{1}{2} (\vec{p}_2 - \vec{p}_3)$$

$$\vec{q} = \frac{1}{\sqrt{3}} \left( \vec{p}_2 + \vec{p}_3 - \frac{\vec{p}_1}{2} \right)$$  \hspace{1cm} (4)

and the direction $\hat{n}$ of the incoming neutron in the laboratory frame $\vec{p}_L = p_L \hat{n}$. It is worth noticing that the Jacobi momenta $\vec{p}$ and $\vec{q}$ thus defined are invariants in any Galilean transformation of coordinates and take consequently the same value when computed in the laboratory (RL) or in the center of mass (RCM) reference frame.

To express the break-up cross section we will chose the incoming energy $T_L$ and the four scalar variables:

$$T_L, \quad \Theta_b = \arctan \left( \frac{q}{p} \right), \quad \hat{n} \cdot \hat{p}, \quad \hat{n} \cdot \hat{q}, \quad \hat{p} \cdot \hat{q}$$ \hspace{1cm} (5)

The quantity $\Theta_b$ is called the break-up angle and measure the relative energy distribution between the fragments.

In the elastic channel, the quantity $\frac{\vec{p}_2 + \vec{p}_3}{2}$ can be identified with the scattered deuteron momenta, $\vec{p}$ becomes an internal variable and the corresponding cross section – which can be considered as a particular case of the break-up case – is characterized by the two kinematical variables

$$T_L, \quad \hat{n} \cdot \hat{q}$$  \hspace{1cm} (6)

We will describe in what follow the numerical method we have used to compute both the elastic and break-up cross sections, having as the only input a given nucleon-nucleon interaction.

### 2.2 The formalism

The n-d reaction is considered as a three particle problem for nucleons interacting via pairwise potentials $\hat{V}_i \equiv V_i(|\vec{r}_j - \vec{r}_k|)$ and is solved by means of the Faddeev equations \[2\]. They consist on a set of coupled equations for the so called Faddeev amplitudes $|\Psi_i>$

\[
\begin{align*}
(E - \hat{H}_0 - \hat{V}_1)|\Psi_1> &= \hat{V}_1(|\Psi_2> + |\Psi_3>) \hspace{1cm} (7) \\
(E - \hat{H}_0 - \hat{V}_2)|\Psi_2> &= \hat{V}_2(|\Psi_3> + |\Psi_1>) \\
(E - \hat{H}_0 - \hat{V}_3)|\Psi_3> &= \hat{V}_3(|\Psi_1> + |\Psi_2>)
\end{align*}
\]

where $\hat{H}_0$ denotes the intrinsic three-body free Hamiltonian. These equations are equivalent to the Schrödinger one but allows a proper treatment of the 3-body scattering problem. The total three-body wavefunction $\Phi$ is given by

$$|\Phi> = |\Psi_1> + |\Psi_2> + |\Psi_3>$$
In the case of identical particles, the three Faddeev amplitudes are related to each other by the permutation operators $P^\pm$. The system (7) is formulated in terms of one of the amplitudes, say $\Psi \equiv \Psi_1$, and reduces to a single equation

$$\left[ E - H_0 - \hat{V} \right] |\Psi> = \hat{V}(P^+ + P^-)|\Psi>$$

(8)

with $\hat{V} \equiv \hat{V}_1$ the unique interaction potential and the wavefunction obtained by

$$|\Phi> = (1 + P^+ + P^-)|\Psi>$$

Equation (8) can be solved in configuration space by projecting it on the set of Jacobi coordinates associated with the amplitude $\Psi_1$

$$\vec{x} = \vec{r}_2 - \vec{r}_3$$
$$\vec{y} = \frac{2}{\sqrt{3}} \left( \frac{\vec{r}_2 + \vec{r}_3}{2} - \vec{r}_1 \right)$$

(9)

The are the canonical conjugate of the Jacobi momenta introduced in the previous section – eq. (4) – and are displayed in Fig. 2.

\begin{center}
\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2.png}
\caption{Jacobi coordinates and momenta used in solving equation (10). They are defined in eqs. (4) and (9).}
\end{figure}
\end{center}

It takes then the form of a partial differential equation on $R^6$

$$[E - H_0 - V(x)] \Psi(\vec{x}, \vec{y}) = V(x)(P^+ + P^-)\Psi(\vec{x}, \vec{y})$$

(10)

where

$$H_0 = \frac{\hbar^2}{M} (\Delta_{\vec{x}} + \Delta_{\vec{y}})$$

and

$$\Psi(\vec{x}, \vec{y}) = |\vec{x}, \vec{y}, \Psi>$$

is the projected amplitude. Notice that a non local coupling is induced by the permutation operators on the right hand side of (10).

In order to solve equation (10), the following boundary conditions [3, 4] must be implemented

$$\Psi(\vec{x}, \vec{y}) = \phi_d(x)f_e(T_L, \theta_e)e^{ik\vec{q}\cdot\vec{r}} + A_b(T_L, \theta_e, \theta_1, \theta_2, \Theta)\frac{e^{ik\rho}}{\rho^{5/2}}$$

(11)

were $\phi_d(x)$ is the deuteron wavefunction and $f_e(T_L, \theta_e)$ and $A_b(T_L, \theta_e, \theta_1, \theta_2, \Theta)$ are respectively the n-d elastic and break-up amplitudes we are interest in. They are extracted from the solution of (10) in the asymptotic region.
This solution has been obtained numerically by means of the standard methods used in the Few-Body problems. They are based on a spline expansion of the Faddeev amplitudes which transform the set of partial differential equations into an homogeneous linear system \[5, 6\].

As discussed in the previous section, these amplitudes depend on the incoming neutron laboratory energy \(T_L\), and the four angles denoted by

\[
\begin{align*}
\theta_e &= \hat{n} \cdot \hat{q} \\
\theta_1 &= \hat{n} \cdot \hat{p} \\
\theta_2 &= \hat{p} \cdot \hat{q} \\
\Theta &= \arctan \frac{p}{q}
\end{align*}
\]

where \(\hat{n}\) is the direction of the incoming neutron.

The elastic cross section is given by

\[
d\sigma_e = \left| f_e(T_L, \theta_e) \right|^2 \frac{9}{4m p_L} d\vec{p}_1 d\vec{p}_2 \delta(\vec{p}_1 + \vec{p}_2 - \vec{P}_i) \delta(E_f - E_i) \tag{13}
\]

where \(\vec{P}_i\) is the total momentum in the initial state (\(\vec{P}_i = \vec{p}_L\) in the laboratory frame), \(E_i\) and \(E_f\) are respectively the total energies on the initial and final states appearing in (11).

In the center of mass frame, \(\vec{P}_i = 0\) and one can show that

\[
\frac{9}{4m p_L} d\vec{p}_1 d\vec{p}_2 \delta(\vec{p}_1 + \vec{p}_2 - \vec{P}_i) \delta(E_f - E_i) = d\Omega_{\hat{q}}
\]

where \(\Omega_{\hat{q}}\) is the solid angle around direction \(\hat{q}\). Then one gets the usual expression for the elastic differential cross section

\[
\frac{d\sigma_e}{d\Omega_{\hat{q}}} = \sigma_e(T_{lab}, \theta_e)
\]

with \(\sigma_e(T_{lab}, \theta_e) \equiv \left| f_e(T_{lab}, \theta_e) \right|^2\).

The break-up cross section has the form

\[
d^3\sigma_b = \frac{1}{8\pi} \frac{\hbar^2}{m} \frac{K_3}{k_{cm}^3} |A_b|^2 d\vec{p}_1 d\vec{p}_2 d\vec{p}_3 \delta(\vec{p}_L - \vec{p}_1 - \vec{p}_2 - \vec{p}_3) \delta(E_f - E_i) \tag{14}
\]

where momentum \(K_3\) is related to the total energy \(E_3\) of the three nucleon system in the center of mass frame

\[
E_3 = \frac{K_3^2}{m}
\]

\(k_{cm}\) is related to the momentum \(\vec{q}\) by \(k_{cm} = \frac{2}{\sqrt{3}} q\) and to the center of mass kinetic energy by

\[
T_{cm} = \frac{\hbar^2}{m} q^2 = \frac{3}{4} \frac{\hbar^2}{m} k_{cm}^2
\]

and \(E_i(E_f)\) are the total energies on the initial(final) states in (13).

3 Comparison with experimental results

The only input in our calculations is the NN potential. We have considered three different interaction models: the so-called semi-realistic (MTI-III) which has no any theoretical ground but give a good description of low energy NN data and two realistic ones (AV18...
and INOY) which are, at least partially, based on a one-boson exchange theory and
describe the NN with a high degree of accuracy.

The semi-realistic MT I-III interaction [7] is given by a simple sum of two Yukawa
potentials, restricted to S-waves only but accounting for the spin-dependent term. Despite
his bare simplicity this interaction reproduces reasonably well the bound states and low
energy scattering observables of the A=2, A=3 and A=4 nuclei, even without three-
nucleon forces [8, 9, 10]. It however fails in describing processes where higher partial
waves are involved.

As realistic NN interactions we have used the Argonne AV18 [11] and INOY [12]
potentials. They have both a much more complex spatial and operator structure and
depend on a large number of parameters (∼ 40) which are fitted to describe almost
perfectly the two-nucleon scattering data. The AV18 is a local potential containing the
pion-exchange tail plus the full ensemble of operators allowed by symmetry to describe
the intermediate and short ranges part of the interaction. However, in order to provided
a good description of some A = 3 and A = 4 zero energy observables (like e.g. the nd
J = 1/2 cross sections) the inclusion of three-nucleon forces is required. The strength
and form of these three-body forces depend on the two-body model they supposed to
complete; together with Argonne AV18 potentials we have considered the so called Urbana
UIX model [13]. The INOY potential superposes a local one-pion exchange tail with a –
purely phenomenological – strongly non-local structure inside some internuclear distance
Rc ≈ 1.5 fm and reproduces well, alone, the overall low energy dynamics of 3- and 4-
nucleon states.

The results for the elastic differential and integrated cross sections are given
respectively in Figs 3 and 4. For the differential cross sections (Fig 3) only the AV18
(solide red line) and MT I-III (dashed blue lines) are displayed. The agreement of AV18
with the experimental points is almost perfect and the differences with the simple MTI-III
model are very small, visible only in the backward cross section. The integrated elastic
cross sections are given in Fig. 4. At zero energy the three models differ each other by
≈2% due to their differences in the nd scattering lenghts. These quantities have been
calculated by several authors [14, 15] and are summarized in Table I. As one can see the
quartet (J = 3/2) value is one order of magnitude greater than the doublet (J = 1/2) one
and when computing the cross sections the quartet channel is furthermore enhanced by
a larger statistical factor. The low energy nd scattering is thus dominated by the J = 3/2
observales, which turn to be not sensible to the three-nucleon forces. The MTI-III slighty
overestimates (by 1%) the experimental quartet scattering length while both AV18 and
INOY are equal to each other and in full agreement with data. One can also remark that,
in absence of UIX three-nucleon forces, the doublet value of AV18 sizeably overestimates
the physical one. These facts explain the behaviour of the low energy cross sections
displayed in Fig. 4. It is worth noticing however that the three considered models are all
still compatible with the existing – unfortunately not very accurate – data for E below
10 MeV.

The results of the differential and integrated break up cross sections are displayed
respectively in Figs 5 and 6. We have presented in Fig. 5 the neutron energy spectra
\( \frac{d^2\sigma}{dE d\Omega} \) of the breakup reaction \( ^3H(n,2n)^3H \) at neutron incident energy of 14.1 MeV and
different angles [16]. As one can see the MTI-III model reproduces well the data. The
integrated breakup cross section as a function of the laboratory kinetic energy displayed
in Fig 6 is also well reproduced by all models up to E ≈ 15 MeV although beyond this
energy, MTI-III suffers from its lack of P-wave interaction.

The total (elastic plus break up) cross sections are given in Fig 7. This quantity,
Figure 3: Elastic differential n-d cross section using AV18 (solid red lines) and MT I-III NN (dashed blue lines) potentials is compared to experimental results taken from [17].

of crucial importance in the Monte Carlo simulations, is however dominated by the elastic part and do not deserve additional comments.

Among the deuteron cross sections, the only one that we have not computed in this work is the neutron capture. This cross section is however needed in the Monte Carlo simulations described in next section. In order to fill this lack, we have taken this cross section from the ENDF/B-VII library [18]. It is displayed in Fig 8 and – in order to evaluate a systematic error – it has been compared with the same results given by the JENDL-4 library [19].

In summary, one can see that AV18 and INOY potentials are in perfect agreement.
both for the elastic and for break-up cross sections. They acurately reproduce the bulk of experimental data, except maybe for some particular break up geometries. This is a general result for any realistic interaction model, which can accurately reproduce the two-nucleon scattering data. Indeed, due to the large deuteron size, the low energy n-d scattering cross section is only sensible to the well controlled long-range part of the two nucleon interaction and is little affected by its short range off-energy shell structure, which differs for realistic models. On the contrary the MT I-III potential underestimates the experimental total cross sections starting from $E \approx 15$ MeV due to the absence of P-wave contribution.

### 4 Heavy water benchmarks

In this work we study the possibility of using the theoretically obtained n-d cross sections in the nuclear facilities simulations. The validity of the various nuclear data libraries as well as the propagation codes are usually tested by trying to reproduce the results of the specially designed Benchmark Experiments. The heavy water benchmarks, being strongly sensitive to the n-d scattering, constitute the testground we are looking for.
Table 1: Neutron-deuteron (nd) scattering lengths (in fm) calculated using MT I-III, AV18 (+UIX) and Doleschall (INOY03) potentials.

|                  | $^2a_{nd}$ (fm) | $^4a_{nd}$ (fm) |
|------------------|-----------------|-----------------|
| MT I-III         | 0.702           | 6.44            |
| INOY03           | 0.523           | 6.34            |
| AV18             | 1.26            | 6.34            |
| AV18+UIX         | 0.595           | 6.34            |
| Exp.             | 0.65±0.04       | 6.35±0.02       |

Figure 5: Neutron energy spectra $\frac{d^3\sigma}{dE\,d\Omega}$ of the breakup reaction $^3H(n,2n)H$ at neutron incident energy of 14.1 MeV and different angles [16] using MT I-III NN potential

We will describe hereafter the technical details of the benchmarks that we have tried to reproduce.

4.1 Description of selected benchmarks

The description of all the benchmarks we have considered in this work, is taken from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICS-BEP Handbook) [20]. These benchmarks – which concern only experiments with deuterium – are extracted from two different parts of this handbook: from the Part II entitled ”Highly Enriched Uranium (HEU)” and from the Part IV denoted ”Low Enriched
Figure 6: Integrated nd break-up cross section using AV18, MT I-III and INOY NN potential

Figure 7: Total (elastic + breakup) n-d cross section using AV18, MT I-III and INOY NN potential

Figure 8: Capture cross section from ENDF/B-VII and JENDL-4 evaluations

Uranium systems (LEU).

Each of these two parts is in its turn separated into four sections, according to
the physical form of the fissile material. For the deuterium experiments we are interested on, the fissile material can be in form of metal (MET), compound (COMP) or solution (SOL). Moreover, each of these four sections is subdivided into fast (FAST), intermediate (INTER), thermal (THERM), and mixed (MIXED) spectra systems, depending on the neutron energy range at which the majority of the fissions occur.

In order to investigate the influence of the n-d cross section – described in previous section – in the simulation codes, we have considered the benchmarks proposed by the ICSBEP Handbook: they consist in 45 experiments from Part II (HEU) and 35 from Part IV (LEU). These experiments provide a consistent basis for evaluating the impact of the n-d cross sections on the reactivity. We will give in what follows, a short description of each type of experiment. A more detailed analysis can be found in [20].

4.1.1 Highly enriched Uranium dioxide cylinders immersed in mixtures of light and heavy water (HCM002)

In this series, 23 critical experiments were performed in 1985 at the Solution Physics Facility of the Institute of Physics and Power Engineering (IPPE), Obninsk, Russia. For the benchmark numbers 1, 4, 5, 8 and 9, the measurements were made using 19 highly enriched uranium cylinders (with diameter 8.3 cm) immersed in light water, whereas three different mixtures of light and heavy water were used for the other cases. A thick bottom reflector of light water was used in all the 23 critical experiments, while in fourteen of them an additional lateral light-water reflector was employed. These experiments have been originally denominated as HEU-COMP-MIXED-002 in [20]. The abbreviation HCM002 is used in our figures.

4.1.2 Cylindrical experiments using HEU plates reflected by lithium deuteride (HMF063)

The Comet Universal Critical Assembly Machine was used to perform a series of HEU critical experiments in 1955 at Los Alamos Scientific Laboratory. The cylindrical assemblies were composed of plates of HEU metal, with 2.54 cm thick reflector of $^6\text{LiD}$ and $\text{LiD}$. These experiments have been originally denominated as HEU-MET-FAST-063 in [20] and are denoted by HMF063 in our figures.

4.1.3 Reflected uranyl-fluoride solutions in heavy water (HST004)

They consist of six experiments in which heavy-water reflecting spheres of uranyl-fluoride have been used. The atomic ratio of deuterium to $^{235}\text{U}$ ranged from 34 to 430. The denomination used in [20] is HEU-SOL-THERM-004 and has been abbreviated as HST004 in our figures.

4.1.4 Unreflected cylinders of Uranyl-Fluoride solutions in heavy water (HST020)

In this benchmark, five assemblies of bare cylinders containing a ratio of deuterium to $^{235}\text{U}$ varying from 230 to 2080 were considered. The denomination used in [20] is HEU-SOL-THERM-020 and corresponds to HST020 in our figures.

4.1.5 RB reactor (HCT017, LMT001, LMT002, LMT015)

An uranium heavy water critical assembly, known as the RB reactor, has a core made of metal uranium fuel elements which are displayed in an aluminum cylindrical tank filled with heavy-water moderator and reflector.
The core of this reactor may vary according to the structure and type of its constituent elements (natural or enriched metal uranium, placed in square lattices with various pitches) and give rise to the following configurations:

- **Lattices of 80%-enriched Uranium in heavy water (HCT017)**
  Lattices of fuel elements – having the form of two concentric cylinders of 146.9 cm height and inner/outer diameters equal 3.1 cm/3.5 cm respectively – are used. The outer cylinder is filled with uranium enriched up to 80%, while the inner one is filled with heavy water when it is immersed in the container. The number of fuel elements may be varied. The experimental sequence is denominated as HEU-COMP-THERM-017 in [20] and abbreviated by HCT017 in our work.

- **Natural-Uranium rods in heavy water (LMT001)**
  The reactor core is made up of 208 metallic natural-uranium rods placed in a square lattice pitch of 12 cm and immersed in a cylindrical tank of aluminum filled by heavy-water. The denomination in [20] is LEU-MET-THERM-001 and is abbreviated as LMT001 by us.

- **Lattices of 2%-enriched Uranium in heavy water (LMT002)**
  The same as (HCT017) cases but the cylinder height may be varied and the uranium is enriched up to 2% only. It is denominated as LEU-MET-THERM-002 in [20] and abbreviated as LMT002 in this work.

- **Fuel assemblies substituted in lattices of 2%-enriched Uranium (LMT015)**
  This core allows the use of several 2%-enriched metallic uranium elements. The fuel rods have the same cylindrical shape but may have void cavity or may be filled with heavy-water. A total of 22 criticality experiments were carried out in three series with different number of fuel elements and with or without void cavity. Two series of 7 criticality experiments in each run were performed. The heavy water contained 1.50 % (molar) fraction of light water. The fuel elements were placed in a square lattice pitch of 8 cm for the first run and 16 cm for the second one. The third run was made up of fuel rods placed in a square lattice pitch of 16 cm and immersed in heavy water with 0.73 % (molar) fraction of light water. The denomination in [20] is LEU-MET-THERM-015 and is denoted by LMT015 in this study.

5 **Results of simulations**

In this section, we present the results of the multiplication factor $K_{eff}$ computed using the nd cross sections described in Section 3. To this aim we have built three new evaluations (in ENDF-6 format) of the deuterium cross sections corresponding to the different NN interactions that we have investigated: MTI-III, AV18, INOY.

The results of our evaluations for the selected benchmarks have been compared with those given by the international libraries.
5.1 Monte Carlo calculations

The ICSBEP Handbook contains the input listings for each experiment to implement the Monte Carlo simulation MCNP5 [21] code in order to calculate the multiplication factor $K_{\text{eff}}$.

The input may be slightly modified to account for the various nuclei described by the libraries. The nuclear cross sections, apart the nd one, are taken from the ENDF/B-VII library.

The total computing time for the 90 selected experiments is approximately 16 hours on 48 processors to achieve a standard deviation less than 25 pcm for each benchmark.

5.2 Thermal scattering laws $S(\alpha, \beta)$

Although this article is not devoted to discuss the thermal scattering laws, commonly denoted $S(\alpha, \beta)$, it is necessary to take them into account in the simulations. Thermal effects have been simulated using the $S(\alpha, \beta)$ taken from the libraries ENDF/B-VII and SAB2002 [22].

The sensitivity study of the deuterium thermal scattering laws is presented in Fig. 9. The multiplication factors calculated using the SAB2002 data are slightly lower than those using ENDF/B-VII and are in a slightly better agreement with the experimental results, especially for HCT017, LMT002 and LMT015 cases. This fact led us to chose the SAB2002 scattering laws all along this study.

5.3 Deuterium evaluation from international libraries

Many recent nuclear data libraries contain an evaluation of the deuterium cross sections. The most recent ones are: the American ENDF/B-VII, the Japanese JENDL-4 and the Chinese CENDL-3.1 [23].

These evaluations provide a complete representation of the nuclear data needed for simulating the neutron transport over an energy range which varies from $10^{-11}$ to 150 MeV in the American library and from $10^{-11}$ to 20 MeV in the Japanese or Chinese ones. The elastic and total n-d cross sections coming from these recent nuclear data libraries are given respectively in Figs 10 and 11. The American and Chinese evaluations of the elastic and total n-d cross sections are identical in all the energy range and differ slightly from the Japanese one below 1 MeV, as can be seen in these Figures.

In Fig. 12 we compare the multiplication factors calculated using the MCNP5 code with the deuterium cross sections taken respectively from ENDF/B-VII (cyan stars), JENDL-4 (red circles) and CENDL-3.1 (blue triangles); as indicated above all the other nuclear cross sections are taken from the ENDF/B-VII library and $S(\alpha, \beta)$ data is imported from SAB2002. In such a way, it is easier to compare the different evaluations. The three deuterium evaluations lead to a systematical underestimation of $K_{\text{eff}}$ values, from about 0.2 to 2.0 %, provided by the HCM002 benchmark measurement.

The ENDF/B-VII evaluation of the deuterium cross sections provides systematically the lowest values whereas the CENDL-3.1 evaluation provides the highest ones; the JENDL-4 result is in between. The largest variation occurs for the HST004 and the HST020 benchmarks.
Figure 9: Comparison of criticality calculations when the thermal scattering laws $S(\alpha, \beta)$ are adapted from ENDF/B-VII [18] (red circles) and SAB2002 [22] (blue triangles) libraries.
5.4 Our new evaluations of the deuterium cross sections

We have built a new deuterium evaluations inserting the cross sections obtained by solving the Faddeev equations with the selected NN potentials. The $K_{\text{eff}}$ values corresponding to the different nucleon-nucleon interactions are presented in Fig. 13. The MTI-III results are indicated by cyan star symbols, AV18 by filled red circles and INOY by filled blue triangles. They are compared to the experimental results of the benchmarks (hachured vertical bars). Notice that for some particular configurations of the HCM002 series (e.g. colons 1,4,5,8,9 starting from left) the three potentials gives identical results. They correspond to the absence of deuterium in the corresponding benchmark but they have been nevertheless included in our simulations as a consistency check.

As a general remark we see that the MT I-III calculations provide always higher reactivities, a direct consequence of its slightly overestimation of the low energy nd cross sections (see Fig 4). Except for the HCM002 series – where the disagreement is slightly reduced – the MTI-III reactivity values are above the experimental results for most of the examined benchmarks. Apart from this particular series, the agreement is systematically improved when using realistic nucleon-nucleon interaction, such as AV18 or INOY. The results displayed in Fig. 13 tend to favour INOY with respect to AV18 interaction, probably due to its non requirement of three-nucleon forces (see results on Table I). This fact demonstrates the importance of a realistic description of the n-d scattering.

We would like to notice however that none of the potentials is able to describe satisfactorily the whole set of benchmarks. A systematic disagreement at the level of 1% exists for some particular configurations of the HCM002, HST020 and LMT015 series which is difficult to attribute to a default of the interaction. The only possible explanation concerning the deuterium data is to be search on the capture cross section or in the thermal scattering laws. An inconsistency of the benchmark themselves cannot be excluded. Is worth noticing for instance that even in absence of deuterium (e.g. colon 1 from HCM002) the simulations cannot reproduce well the experimental result.
Figure 12: Sensitivity of the criticality calculation to the n-d cross sections taken from the different libraries: ENDF/B-VII (cyan stars), JENDL-4 (red circles) and CENDL-3.1 (blue triangles).
Figure 13: Multiplication factors $K_{eff}$ obtained in Monte-Carlo simulations using the nd cross sections given by different NN interaction models: MT I-III (cyan star symbols), AV18 (red circles) and INOY (blue triangles). They are compared to experimental results of selected benchmarks (hachured vertical bars).
Finally we have compared in Fig. 14 the reactivity obtained using the INOY deuterium cross sections (red circles) with the calculations based on the international library cross sections CENDL-3.1 (cyan stars) and JENDL-4 (blue triangles). In general, the INOY results settles in between those of these two libraries. We conclude from that, that the evaluations based on n-d cross sections obtained from \textit{ab initio} nuclear physics calculations are of the same quality than those provided by the best established international library. It would be interesting to perform similar studies by computing other interesting quantities in the neutron transport simulations.

![Diagram showing sensitivity of criticality calculation to n-d cross sections input](image)

**Figure 14:** Sensitivity of the criticality calculation to the n-d cross sections input: the \textit{ab initio} INOY results (red circles) are compared to those given by the CENDL-3.1 (cyan stars) and JENDL-4 (blue triangles) libraries.

### 6 Conclusion

The aim of this paper was to check the validity of \textit{ab initio} nuclear calculations in the integral experiments involving critical benchmarks.

By solving the Faddeev equations in configuration space, we have computed the
n-d differential elastic and break-up cross sections using three different nucleon-nucleon interactions (MTI-III, AV18 and INOY). These cross sections have been inserted in a Monte Carlo simulation of neutron transport to obtain the multiplication factor $K_{eff}$.

The results have been compared to some selected experimental benchmark. We have found that the semi-realistic MTI-III potential systematically overestimates the reactivity and that the best agreement is provided by the non local nucleon-nucleon potential INOY. These results fail however to describe accurately the whole set of benchmarks and a systematic discrepancy (of the order of 1%) exists for some particular configurations which is difficult to attribute to a default of the interaction.

The results obtained by the *ab initio* INOY potential have been compared with the calculations based on the international library cross sections and are found to be of the same quality. It would be interesting to perform similar studies by computing other quantities which are relevant in the neutron transport simulations.

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