MONTE CARLO SIMULATION OF MIGRATION OF FUSION PLASMA NEUTRONS - OPTIMIZATION AND TRAPS

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We recall some of the sensitive points and stages in random walk of neutron, frequent solutions and their consequences on quality and duration of MC neutronic and photonic simulations. We present some unconventional approaches we developed to precisely meet the double paramount MC goal: maximal probing at minimal variance, whence minimum CPU time. Instead of the traditional ***point*** observation, enhanced probing is used to limit collected random scatter dispersion. Vector probing by ***shower*** (through "*nuclear reaction-channel*" space) and ***drizzle*** (improved sampling throughout space involving even the deepest parts, with region fragmentation allowed) drastically reduces the collected variance. By treating analogically close-collision ***flux-at-a-point*** tallies, the unphysical pole discontinuity at-the-detecting-point is avoided - this allows the study of even within-detector collisions. For deep shielding treatment the use of the two-step Cascade Monte Carlo is recommended as it reproduces from physical considerations the mathematical approach. Making sure to distinguish ***volumetric*** versus ***local*** destructive effects, the latter requiring the use of "statistics of extreme values".

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1. INTRODUCTION

The quality of statistical simulation of neutron migration through material space and the induced effects under study, be they local (*in situ*) or far (as revealed by a detector), can be judged by how fully the concerned material space is probed, and how low is the variance obtained for the values sought. This twin requirement maximal probing with minimal variance is the essence of any Monte Carlo calculation. Ever since the start, MC probing and variance have been conditioned by memory and speed constraints. Computer evolution drastically improved the situation. Yet they still remain an issue, due to ever-increased requirements of quality of simulations of fusion device details. The gigantic codes built in the past, as well as recent, object-specialized codes bargain simplifications (*shortcuts* - that inevitably deform reality) vs. quality of representation to keep simulations in rational financial frame and timely delivery of results. Fusion devices have extended, non uniform (time and space) neutron sources, numerous ports through the structure and blanket and a variety of surrounding materials and devices sensitive to fast or slow neutrons and photon radiation that all need as close to reality a simulation. It is no exaggeration to say that neutronics and photonics of fusion devices is a most challenging MC task among other nuclear related simulations.

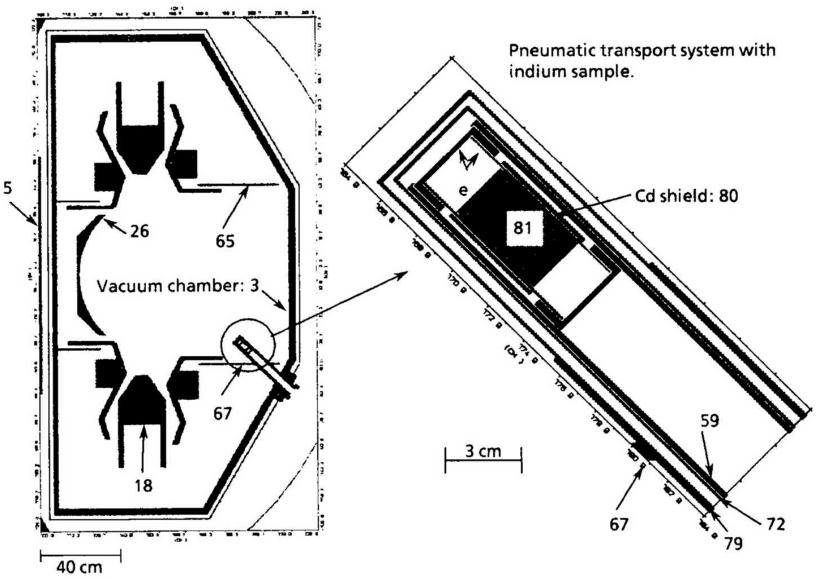
The plague to the required variance precision resides in the occurrence of collisions that result in ***rare-but-strong-events*** (RSE) and explode the variance due to their being out of proportion with the rest of event probabilities. It is folly if one ignores them. A simple solution to "smooth" them out is to increase the number of iterations corresponding to the out-of-proportion ratio, which often turns out to be prohibitive. The situation can become dramatic when any of these RSE events contributes to a narrow energy interval of interest. Another solution, the one we advocate and have adopted [1,2], is to ensure, while probing the required object, collecting each contribution proportionately to its natural importance. This is readily achieved using the approach of which the essence is described below. The method has proved powerful when applied to such different problems as for example, in blanket tritium-breeding evaluations [3], neutron detector calibration in the vicinity of a massive structure, and fast-neutron diagnostics [4], fast-neutron radiography [5,6], even gamma analysis [7], etc.

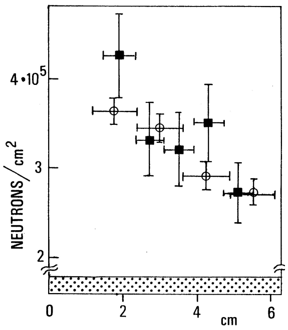
2. MC SIMULATION OF NEUTRON MIGRATION - BASIC REQUIREMENTS

Modern thermonuclear plasma research is concerned, both for project design or experimental diagnostic interpretation, with ever more complex and sophisticated systems accompanied by ever more stringent demands on reliable estimation results. To be useful, the simulation of radiation migration (neutron, gamma) has strict requirements on variance [8] to be less than 40% for feasibility projects, 20% for design, 10% for coding, 5% for testing, 2% for installation, 1% for safety estimates. Naturally, simulations must faithfully reproduce and probe the provided shapes and compositions. The revolutionary developments of computer speed and memory help in conceiving such aims.

Neutron diagnostics at large plasma devices require for the interpretation of the measurements often an accompanying MC simulation. Here the importance of obtaining small variances is far greater in diagnostics than in detection. In fact, in detection a value is measured and the standard deviation error is determined. In diagnostics, as a parameter is varied, one aims to detect the variation in the measured signal. To detect such a variation, the σ_{errors} of the simulated signal must be smaller than half the variation in the signal!

The interpretation of neutron diagnostics for large fusion facilities requires numerical simulation of the full experiment: start from the neutron emission in a plasma with known parameters (either as per project parameters, or experimentally measured on the facility); follow the migration of the neutrons through the complicated structures of the device and the detector; conclude with the response of the detectors used. Naturally, uncertainties and statistical errors at each step of the calculation sum up nonlinearly and determine the overall quality of the simulation.





Neutron flux decrease along nuclear emulsion axis for ASDEX discharge #16911 (collimator-1). Solid squares: measured values, open circles: MC estimation

Fig.1: A poloidal cross-section of ASDEX [1] through the vacuum chamber and the detecting pneumatic transport tube (as seen by the computer). Numbers refer to a selection of parts of the device. Parts shown are

- ***Main section:** 3-ASDEX vacuum chamber, 5-ohmic field coils, 18-divertor, 26-carbon shield, 65 & 67-thin stainless steel shield protecting the divertor chamber.*
- ***Blow-up:** 81-nuclear emulsion or indium sample; 79 & 72-protective tubes; 59-transport tube; (e) transport box.*
- *Nuclear emulsion plate track density of recoils MC-estimated vs. measured on ASDEX shot #16911 [9].*

3. SPACE PROBING IN MC SIMULATION OF NEUTRON MIGRATION

In essence, Monte Carlo (MC) neutron or gamma simulation (of effects on structure, or detectors, or safety hazard estimations) is a probabilistic probing of a given space S_{body} exposed to neutrons emanating from a subspace S_{source}, and registering select information about effects produced either in S_{body} itself at large, or in a restricted subspace S_r (particular sensitive part as detector, insulator, et al.). The aim is to estimate the values of interest with as reduced statistical variance as possible. Values of interest may be ***local*** within the extended S_{body} with direct probabilistically high access by neutrons (such as generation of tritium breading in blankets, transmutation gas-products or induced radioactivity, energy deposition, etc.) or within a ***remote*** space of low probability of direct access to neutrons, due to either small size (as detectors or sensitive parts as insulators et al.) or deeply shielded parts. Naturally, the two necessitate distinct approaches.

To ensure credibility of results the MC should densely cover with stochastic points all of S_{source} , S_{body} and S_r.

1. Source S_{source} is the emission seat of neutrons (or neutron ¨package¨), to be defined each as realistically as feasible: 1) starting *point* position, 2) energy 'E' spectrum (thermonuclear plasmas, plasmas with additional heating, etc., 3) direction of emission '**u**' anisotropy selected, 4) corresponding probabilistic weight 'W'. Sources vary from small sized Plasma Focus emitters[5] , accelerator target source[10], or neutron fission sources (as Californium), to vast tokamaks with sophisticated space emission and varying energy spectra as in case of ion injection, et al. The starting neutron weight is to faithfully reflect the project (as GDT [11]) or experimentally determined probability profiles (tokamaks as ASDEX [12], TEXTOR [13], etc.). When a part of S_{source} has more physical significance for the intended research as per experimental setup (vicinity, collimation, etc.), the split method [14] is to be applied to enhance the influence of the effective part of S_{source}, while respecting the rest of the source, guarantying invariance of the total source emission. In the case of collimator shielded detectors to ensure optimal tally collection and hence variance, one has to distinguish points not in view of the collimator entrance (CE), from those that view directly the entrance at a solid angle Ω_{CE}. Here again the split method is recommended, selecting many more probing small weight neutron-stories are "emitted" into Ω_{CE}, while proportionately fewer but "heavier" ones sent into the

complementary $4\pi-\Omega_{CE}$. In case the emission-point is in-view of the detecting point, to ensure in the correct proportion for contributions of direct and back-scattered fluxes, we use a further split with a neutron story run for half the weight beamed forward into Ω_{CE}. This is followed by another story run with identical all other start parameters, but beamed into the vertex-opposite *anti-beam*-Ω_{CE}; naturally here the complementary stories are beamed into $4\pi - 2\Omega_{CE}$. Thus, the proportionality of scattered to direct contributions is ensured.

2. The whole facility space S_{body} has to be faithfully reproduced. To simulate the Garching tokamak ASDEX [12] or the Novosibirsk GDT neutron source [11] required several hundred structural elemental volumes, each with its proper chemical composition involving several decades of nuclides with an average of half a dozen reaction channels each. TEXTOR used 1157 elemental volumes [13]. All these have to be densely probed.
3. Eventual particularly sensitive parts S_r are to be treated with stochastic tally point-collectors. Detection is particularly sensitive to events close to, and unshielded from the detector - whence the importance of close collision. For detector simulation, for each neutron story a stochastic detecting point is selected within S_r , that is to be densely probed.
4. Deeply shielded, as in GTD [11], vital parts require both, special treatment to densely probe them, and need the statistics of extreme-tallies interpretation.

The distinct MC software sets designed to solve each one of the above problems are strongly correlated. The output of the neutron source program serves as input to the neutron migration software, whose output in turn serves as input to the several software programs for simulating the response of the different detectors.

Fig. 1 shows as an example our computer simulation of the poloidal cross-section of the tokamak ASDEX [1] and of the details of the head of our transport system which was used to expose as well activation samples (e.g. Indium) as nuclear emulsion plates [9] near the plasma boundary. As an example of the results the simulated and measured values and their variance of the neutron flux in an emulsion is shown. This flux, as per figure, decreases along the emulsion axis due to neutron absorption by about 25%.

4. MC SIMULATION OF NEUTRON MIGRATION – CLASSICAL NEUTRON TALLY

Due to its zero charge, a neutron (or photon) flies rectilinearly until the next event in space. The MC simulation of neutron ***migration*** [14] follows each ***neutron story*** that extends from emission down to disappearance through an absorption event, or till energy or weight *cut off* below which further simulation is estimated to be of no interest (as in threshold-energy detector studies, or too weak tallies). Event-wise a collided, neutron reacts probabilistically with one of the nuclides at that position, and follows one of the possible reaction channels. Classically, this is recorded locally at the point of event, or observed remotely at the detecting point, with tallying and migration confound and related to points touched upon by migration with the full contribution assigned locally. The neutron then proceeds till the following event with an altered direction (anisotropy selected), energy 'E' (either event defined or spectrum probabilistically selected) and weight 'W' (material attenuated along the flight path 'x' with $dW/W(x) = \Sigma_{nuclide}\, n_{nuclide}(x)\ \Sigma_{channel}\, \sigma_{nuclide,channel}(x)\, dx) = dx/\lambda(x)$ with λ the radiation mean-free-path. At the neutron-story end, the MC registers the *terminal* contribution (usually accessible to an analytical estimation), and a next neutron story is generated. To be credible the simulation should probe, i.e., touch upon as densely as possible all parts of S_{body}. This requires many stories. However, probing probability diminishes with depth away from the source favoring parts directly exposed to the source emission. To obviate to such inconveniences, several solutions had been proposed in the past [14] that force neutron propagation into directions of interest at the expense of other directions.

This classical method yields a single tally per migratory event**.** We shall refer to such tally collection as "***scalar probing"***.

5. IMPROVEMENTS BY VECTOR PROBING OF SPACE AND MATERIALS

Neutron probability of interaction or of probing is low in the following situations.

1. The specimen is thin in size, and the mean-free-path is far greater than the through size of the object. As in Fig.1 the thin protective shields (for light, X-ray, thermal neutron shields) as well as close thin shields installed for other purposes, would lead to rare, lumped, strong contributions totally offsetting the variance of the collected distribution. Indeed, in the Fig.1 illustrative case the thin shields attenuate the neutron fluence passing to the detector by ~25%, while contributing ~16% of the collided fluence arriving at the detector. Here, ***forced-collision*** approach [15] is recommended.
2. The object is small and remote (such as a detector), the ***flux-at-a-point*** estimation method of uncollided flux has been devised [16].
3. Regions are highly shielded hence poorly accessible to neutrons as per project design [11].
4. The encountered nuclides are rare, and reaction channels not predominant.

Whenever any such rare event occurs, the tally is out of proportion with respect to other tallies, and the relative variance explodes, requiring a high number of stories to smooth the resulting discontinuity.

To offset the drawbacks of scalar probing we advocate and use ***vector probing*** through space (***drizzle*** [1]) and nuclide reaction-channels (***shower*** [1]), i.e. two additional splitting methods [14]. Both methods have been described earlier [1] and are here only briefly recalled. Indeed, in defining migration, all nuclides and channels are considered to determine the collision event that leads to the next migration-step of the neutron story, and the tally at the point of event, or of detection.

Vector probing through all nuclides and reaction channels at each point, ensures the tallying of all the ***shower*** of events proportionately to their probabilities, by considering in a material all nuclide components, accounting for different product of isotopic abundance $n_{nuclide}$ and reaction-channel cross section $\sigma_{nuclide,channel}$. This avoids out of scale contributions, ensuring a smoothly converging variance collection. By guaranteeing a full probing through all possible nuclear reactions, ***shower*** totally eliminates perturbations introduced by rare nuclear reactions due to trace elements or low cross-section branches.

In selecting the migration event point one determines the absorption attenuation of the neutron flux as it proceeds along its line of flight till the very edge of S_{body}. This constitutes a ***beam*** probing through space even to and across the most deep and remote parts. Along this probing beam, and using the same algorithm as adopted for the neutron migration, by ***vector probing*** a random point of pseudo-event is selected for each traversed absorbing material region (or in case of vast regions, fractions of there of). The fraction of the flux absorbed in each structural element (or sub-element) of the facility, is considered to have its set of shower reactions leading to a distributed ***drizzle*** of contributions through space, all in perfect scale! *Drizzle* is useful in treating material regions with a disproportionately large mean-free-path of radiation – as thin detector protective foils, spaces that stop neutrons only rarely, but when they do, the event leads to intense tallies. The method ensures that the absorbed flux is distributed to each solicited region proportionally to the natural capacity to interact.). Naturally, such a drizzle approach uses the ***forced-collision***, which accounts for the fraction of the flux lost at the beam-end, while the remaining flux is distributed proportionately to absorption in each traversed region, be it for local or remote tallying. The drizzle-shower approach is particularly useful to account for thin protective foils around small detectors exposed to the plasma direct radiation. Drizzle's ***beam-probing*** greatly enhances probing of space.

For each collected shower-drizzle tallies the following data are stored:

a) coordinates of the points of emission, events and detection for each story,
b) time of emission or event, necessary for time-of-flight detection or other time-resolved studies,
c) weight probability, or flux, and energy of the neutron contribution arriving at the detection point,
d) identifiers for the origin of neutron re-emission as collided nuclide and reaction branch, tokamak structural element (region), and the partition of space as observed by the detector (zone), etc.

This tally database allows identifying quantitatively the contribution of different parts of S_{body} or nuclear contributors, such as the different fluence components (direct or scattered; structural part in which scatter occurred, etc.), spectra and fluence of neutrons arriving at the detector. The tally database also serves to determine the collimator response function, as well as that of the detector using post processing software. Example of such software are ACTIN for indium-activation diagnostics [4,13,17], NEPMC for nuclear emulsion plate (NEP) measurements of proton recoil parameters (track length, angle, proton energy, accounting for track strangling, emulsion thickness variation) as was applied in [4,9, 13,17].

6. CLOSE COLLISION SIMULATION

Detection simulation has long been plagued with RSE occurring close or within the detector collecting the tally.

Close collisions are unavoidably part of a true detector simulation. Indeed, the reduction of the detected intensity by surrounding material structures and attenuation due to distance, limits the space of origin of the intense tally contributors to but a few mean-free-paths around the detector. Thus paramount is the attention to events within their close vicinity. The flux-at-a-point as per Kalos-expression [15] intrinsically contains the $^1/4\pi d^2$ singularity. To tackle close-collisions several treatments have been proposed [16], as the *once collided* estimator and other similar treatments.

We chose an analogic approach. To record flux information in a small subspace S_r we estimate the fraction of the scatter of each event into 4π space that reaches per cm^2 at S_r [$\delta\Omega/4\pi = ½\,[1\text{-}d/(d^2+1/\pi)^{½}]$]. Such estimation is perfectly regular (with no singularity) and hence fit to tackle even the very close events (see for instance [9]). But most important it reproduces the physical reality that no more than ½ of the emanating flux may be gathered at any surface, the other half traveling the opposite direction and hence is lost. The unphysical pole discontinuity at-the-detecting-point is thus avoided, and the study of even within-the detector (as in nuclear emulsion detection simulations) becomes possible [9]. The treatment of very close events is fundamental to correctly simulate neutron diagnostics.

7. HEAVILY SHIELDED PARTS AND THE TWO-STEP CASCADE MC

Damage effects in heavily shielded parts $S_{HeavySh}$, require close attention. Indeed, heavy shielding implies, as per project intent, that only a negligible part of neutrons reach those sensitive parts. Such parts receive mostly events attenuated in energy and flux intensity, with very few but very damaging exceptional high-energy arrivals. To correctly simulate such a situation a two-step Cascade Monte Carlo [2] is recommended. The method reproduces from physical considerations the mathematical approach [18]. It consists of an initial MC simulation in which the deeply-shielded part surface serves as a collector of all arriving beamed (onto the probing point selected within S_r for that story) neutrons (defined each in weight, energy, direction) while the $S_{HeavySh}$ volume is assumed normally absorbing but non-collisional.

In the second step of the cascade $S_{HeavySh}$ becomes normally colliding to all effects, while the space around it, S_{body}-$S_{HeavySh}$ is either dropped if S_{body} is singly connected, otherwise considered collisionless for economy of computation time. Only a ***skin*** is retained to be able to account for reentering neutrons that scatter out of $S_{HeavySh}$ [2]. Each of the registered neutron contributions now acts as the neutron-story start, and the MC is run normally. Yet, in recording destructive effects, a strong distinction is to be made between ***volumetric*** versus ***local*** effects, the latter requiring the use of "statistics of extreme values" [11]. Indeed, while energy deposition is an integrated value that is mediated with a majority of low values adding to very few strong contributions, damage to an insulator or superconductor is a local effect and destruction occurs with single local damage. This implies that in estimating the survival life of a critical part, statistics ought to be carried out on collected "extreme values". Thus the second cascade is repeated several times, collecting a sufficient number of extreme values, whence the statistics of these extreme values serves to determine the effective survival time.

8. CONCLUSION REMARKS

A classical *analogical* simulation run requires usually great many thousands of MC stories. The introduction of some evaluation methods as flux-at-a-point, forced-collisions, greatly reduces the required number of story runs. The analogical flux-at-a-point consents the treatment of very close events. Drizzle and shower splitting, rend conceivable numerical experiments of high complexity and sophistication, that otherwise would be inaccessible due to the time they would require (in spite of the ever faster computers). This is due to their capacity of collecting tallies with rapidly converging random statistical dispersion to the experimental values due to their greatly enhanced probing of space, of material nuclides, of reaction-channels, all gathered proportionately to their relative natural contributions.

Drizzle beam probing is more powerful than regional biasing when applied to tritium-breeding blankets of thermonuclear facilities or in estimating safety hazards from radioactivity hands-on after shut down of the tokamak. For the latter we recommend full drizzle and shower biased to the reactions of interest. The two-step cascade MC is a technique that consents tackling *extreme* experiments.

Both our VINIA-3DAMC (see for instance [4]) and 3DMCSC-RWR (see [7]) software complexes have drizzle, shower, and the analogical close-collision estimator as functional and integral parts. They yield results in absolute units referred to the total measured or project yield of the facility, and do not use any parameters or normalization factors.

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