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Title:

THE ACCELERATION TECHNIQUES USED IN THE MONTE CARLO CODE MCBEND

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ABSTRACT

The paper describes three of the acceleration techniques available in the Monte Carlo code MCBEND\textsuperscript{1}, which has been developed by AEA Technology. The philosophy of accelerating MCBEND is based on splitting and Russian roulette, with the geometry model being overlaid by an orthogonal splitting mesh and energy dependent importances being specified for each spatial interval. The values of importance are usually generated by a diffusion calculation run in adjoint mode which is performed as an integral part of the MCBEND run. This acceleration method works very well for calculations involving penetration through bulk material or which include a moderate degree of radiation streaming; but for problems in which streaming is the dominant mode of penetration this approach can be inadequate. Two new capabilities for enhancing the acceleration of MCBEND in such situations have been introduced. The first is designed to improve the efficiency of the analysis of collimated systems, and involves the addition to the normal Monte Carlo tracking of a deterministic - or “forced” - flight from collision sites to the collimator. The second capability caters for the more general streaming calculation and involves biasing the angle of scatter at a collision so that particles will preferentially scatter into important directions along the streaming path. The paper describes the functionality of the above capabilities, gives examples of their use, and discusses the gains in calculational efficiency achieved.

I. INTRODUCTION

Over the last decade or so, the Monte Carlo method has moved from a reference method against which more approximate calculations could be tested, to the first choice for performing many shielding design and assessment calculations ranging from the routine to the extremely complex. Two factors have enabled this progression to occur: increased speed of hardware and greater efficiency of calculation. This report describes the latter as applied to the MCBEND code.

For the vast majority of shielding problems, using Monte Carlo in analogue mode, ie without any variance reduction techniques, would lead to impractically long running times. Various different techniques are used to reduce the statistical error on the Monte Carlo result, the most widespread being the combination of splitting and Russian roulette (S/R). This operates by interrogating the probability of a particle scoring at the detector as it moves through the system, this probability being known as the importance. If the particle is becoming more important (as it gets nearer the detector), it is split into fragments, thus increasing the chances of the particle making a contribution to the detector. Conversely, if the particle is becoming less important, it is subjected to Russian roulette with the possibility of its being killed. This reduces the time wasted in tracking particles which have little chance of scoring. Altering the particle weight to compensate for the S/R process ensures that there is no bias in the calculation. When using a Monte Carlo code, values of importances can be either estimated by the user or derived from an adjoint solution of the transport equation. As the latter calculation can be as time-consuming to perform as a forward Monte Carlo calculation, approximations to the transport equation, eg the discrete ordinates method in a reduced number of dimensions or diffusion theory, are often used to provide importances.

In MCBEND, the importances are specified in an orthogonal mesh superimposed on the model of the system being analysed. Energy-dependent values of importance are usually generated by a diffusion calculation run in adjoint mode, this being performed as an integral part of the MCBEND run with minimal user intervention. This capability, known as MAGIC\textsuperscript{2}, has been extremely successful in producing importance maps for penetration calculations. To further aid the efficiency of the calculation, source sampling in terms of space and energy may be driven by the same importances.

There are, however, several situations where diffusion theory alone cannot provide adequate importances for the acceleration of the Monte Carlo
calculation, namely where a significant amount of streaming is present and, more specifically, in collimated systems. Two capabilities have been developed in MCBEND which are aimed at improving the efficiency of such calculations.

In systems where a gamma-ray detector is protected by a collimator, it is difficult to encourage particles to travel down the collimator using conventional (ie space/energy) importances. The forced flight capability overcomes this problem by tracking particles deterministically from collision sites outboard of the collimator to a geometric interface in the collimator. The particles resume normal tracking on the other side of the interface and travel to the detector.

For streaming calculations in general, it is often only a very small - but very important - fraction of the particles which travel along the streaming path, eg are transported across a region of void to a detector. The population of particles at the far end of the streaming path can be increased by encouraging the particles undergoing collisions in the walls of the void to scatter in preferred directions rather than by simply sampling from the angular distribution given by the nuclear data. A capability has been developed in MCBEND for biasing the angle of scatter so that particles near the boundaries of a void will preferentially scatter in directions determined by a combination of the nuclear data and importances which vary with angle. These importances can be estimated, or calculated using MCBEND run in adjoint mode.

The following sections describe the functionality and operation of MAGIC, forced flight and angular biasing of scatter and demonstrate through a series of applications the benefits to calculational efficiency that can be achieved.

II. AUTOMATIC IMPORTANCE GENERATION

A central feature of any Monte Carlo code for penetration studies is the provision of an efficient acceleration technique. For most calculations MCBEND employs the well-established method of splitting and Russian roulette to encourage particles from remote regions of low importance to reach those of higher importance close to the region of interest. A multigroup importance function is used to represent the energy variation, and data are derived from an adjoint solution of the ADC (adjusted diffusion constant) diffusion equation. This approximates the single energy group transport equation by a two-component diffusion model, the diffusion constants being adjusted to give agreement with ANISN calculations of attenuation through semi-infinite slabs of material. The adjustment compensates for the inaccuracy of diffusion theory at deep penetration.

Prior to the developments described in this paper, it was necessary for the user to perform an adjoint calculation with an independent diffusion code and manually transfer the adjoint fluxes into the MCBEND input data for use as importances. This meant that the user had to set up two different sets of input data for codes with different user images, run two separate calculations, and make sure that the transfer of importances had been done correctly - all of which was burdensome. The process has been automated by including the above functionality as an option in MCBEND by means of what is known as the MAGIC module.

The importance function is specified with respect to an orthogonal mesh superimposed upon the material geometry. The user specifies the mesh in XYZ or RθZ geometry, the mesh spacing taking account of material boundaries and the expected attenuation through the system. As MCBEND uses binary splitting, so that at a splitting surface particles are split into 2n further particles (where 2n is approximately the ratio of the importances either side of the splitting surface), the meshes should ideally be spaced so that the importance from one mesh to the next changes by a factor of two. This is of course unattainable for a multi-dimensional multi-group case, but it has been found that MAGIC is not over-sensitive to the choice of mesh and has been demonstrated to be robust in the hands of even the novice user.

MAGIC determines the composition of the material in each mesh by sampling the material type in the Monte Carlo model at several points in the mesh and smearing the materials accordingly. Regions of void are represented as low-density aluminium. This has been found to be adequate for small voids, with calculations which involve significant amounts of radiation streaming being considered later. The boundary conditions for the diffusion calculation are taken to be black or reflecting depending on the external boundary condition specified in the Monte Carlo model.

The source spectrum for the adjoint calculation is taken to be the first response function specified in the MCBEND input. The position of the adjoint source is identified by flagging the zone(s) of the Monte Carlo model where the results are required. The adjoint diffusion calculation is then performed using the finite difference technique, and typically takes an insignificant amount of the time dedicated to the Monte Carlo calculation. For instance, in a study of the fluence in the pressure vessel of a PWR, which determined various reaction-rates in the PWR cavity to a statistical accuracy of 2%, the solution of the adjoint diffusion equation took less than 1% of the total run time.

An example of MAGIC's application is the calculation by MCBEND of dose-rates outside a TN12 fuel transport flask due to the sources in the fuel.
Figure 1. Neutron, gamma-ray and coupled (n,γ) calculations were required, all of which are catered for by MCBEND and by MAGIC.

![Figure 1 - MAGIC representation of dry fuel transport flask](image)

The fuel, twelve PWR fuel elements in a basket, is contained in a steel flask. Polyester resin between the copper fins on the outside of the flask provide extra neutron shielding, the fins being modelled as a smear. The flask is protected by balsa wood shock absorbers.

Although the arrangement of the fuel in the flask was not azimuthally symmetric, such variation was not required for the importances and an RZ splitting mesh was used, as indicated by the grid in Figure 1. Splitting planes were positioned as described above. As results were required in many positions outside the flask, the adjoint source was positioned in the void surrounding the flask. Even though this is represented by MAGIC as aluminium of density 0.1 g/cm³, which may be expected to lead to convergence problems with the finite difference solution, no problems were experienced regarding the robustness of MAGIC in such a case.

In MCBEND, the neutron and gamma-ray parts of a coupled calculation are performed separately, which means that it is possible to specify different splitting meshes for the two calculations as appropriate for the penetrating properties of the two types of particle. Importances for the first (neutron) stage of the Monte Carlo calculation are determined by a coupled (n,γ) MAGIC calculation so that neutrons are accelerated into positions and energies where they are likely to produce the most important gamma-rays for the second stage.

As a demonstration of MAGIC’s ease of use, the MCBEND input data appropriate to the option are listed below. Given that a response function and splitting mesh would have to be specified whatever means were used to derive the importances, the extra input data runs:

- **CALCULATE** *(an introductory keyword)*
- **TARGETS** (number of zones of interest)
- **ZONES** (zone identifiers)
- **STRENGTHS** (relative importance of each zone)

Keywords are in upper case, parameters to be set in lower case, and comments in italics. The brevity of the input data speaks for itself.

MAGIC’s ease of use, robustness and effectiveness in producing accurate values of importance has made the capability almost universal for accelerating MCBEND calculations involving material penetration, and - as if by “magic” - relieved the user of much of the burden of providing importances for Monte Carlo calculations. It also provides a standard and consistent approach which can be validated for particular applications.

### III. COLLIMATED SYSTEMS

An area where the acceleration of Monte Carlo is difficult to achieve by adjoint diffusion theory alone is the transport of gamma-rays in collimated systems. For example, a typical oil-well logging tool, as illustrated in Figure 2, contains a gamma-ray source and detectors which measure gamma-rays scattered back from the rock formation surrounding the borehole. The tungsten housing for the detector nearest the source has only a narrow opening through which a collimated beam of gamma-rays can reach the detector.

It is very difficult, using conventional S/R, to persuade the gamma-rays to travel down the collimator to the detector. The system does not lend itself to accurate modelling in an orthogonal mesh for the adjoint diffusion calculation, and the transport mechanism is dominated by gamma-rays which scatter in the formation and then undergo a direct flight down the collimator to the detector - a physical process not treated accurately by diffusion theory nor efficiently by Monte Carlo with analogue sampling of scatter. MAGIC can, however, adequately accelerate gamma-rays from the source into the formation, and a new capability (which is currently only applicable to gamma-ray transport) has been developed to improve the efficiency of transport from collision sites in the formation to the detector.

An interface is introduced into the collimator, see Figure 3, and from each collision outboard of this...
interface a particle is transported deterministically to the interface by ray-tracing from the collision site, see Figure 4.

A particle travelling in direction $\Omega$ with energy $E$ is scattered at point $r$. The forced flight process creates a particle on the interface by sampling and weighting in such a way as to give the correct spatial, angular and energy distribution for particles crossing the interface uncollided after scattering from $(r, \Omega, E)$. To simplify the notation in the following analysis, these initial parameters are omitted. The other parameters are as defined in Figure 4.

The crossing point $r'$ is chosen by sampling from a uniform distribution over the interface. This determines the angle of scatter. The energy $E'$ is then sampled from the normal secondary energy distribution for the reaction which occurred at $r$. This distribution may take the special form of a functional relationship between the energy and the angle of scatter.

The particle weight must be multiplied by the ratio of the true probability to the sampling probability. Consider a small area $dA$ surrounding the point $r'$ on the interface. This subdends a solid angle $(\mathbf{n} \cdot \Omega') dA/R^2$ at $r$. The true probability that the scattered particle, without undergoing any intermediate collisions, will cross the area $dA$ with an energy within an interval $dE'$ about $E'$ is given by

$$P = (\mathbf{n} \cdot \Omega') dA p(\Omega') q(E'|\Omega') dE' e^{-\tau(E')}/R^2$$  \hspace{1cm} (1)$$

where $p(\Omega')$ is the angular distribution of scatter, $q(E'|\Omega')$ is the secondary energy distribution for a given scattering angle, and $e^{-\tau(E')}$ is a simplified notation for the attenuation through $\tau$ mean free paths of material between $r$ and $r'$.

The probability of such an event occurring in the forced flight sampling procedure is

$$Q = \frac{dA}{A} q(E'|\Omega') dE'$$  \hspace{1cm} (2)$$
The factor to be applied to the particle weight is therefore given by
\[ F = \frac{P}{Q} = (-n \Omega') A p(\Omega') e^{-\tau(E')}/R^2 \] (3)

If the collision site is close to the interface, there is a danger of \( F \) tending to infinity as \( R \) tends to zero. MCBEND caters for this possibility by using a different sampling technique if the collision occurs within a certain distance of the interface, this distance being determined by examination of the likely weight changes near to the interface.

A particle with its weight altered as above from that of the scattered particle is created at \( r' \) with energy \( E' \) and direction \( \Omega' \). It is then tracked by the normal Monte Carlo process, its chances of reaching the detector having been greatly enhanced. The weight of the gamma-ray at the collision site is not altered, and it proceeds as normal; but to avoid double-counting it is killed if it naturally crosses the interface.

The interface may be circular, elliptical, rectangular or spherical, and there may be more than one. The input data for the common forced flight option of a single circular interface runs:

BEGIN FORCED FLIGHT (introductory keywords)
INTERFACES 1
DISC
(co-ordinates of the centre of the disc, its radius and orientation)

In Figure 3, the interface is shown extending into the tungsten for a short distance so that those particles which just clip the walls of the collimator are included. To reduce inefficiencies due to processing unimportant events, there are extra options allowing the user to specify the domain over which forced flight is permitted, and the probability of a forced flight event may be biased by reference to the importance at the collision site. The use of this method in conjunction with MAGIC has led to an increase in the efficiency of calculation by about a factor 30 over using MAGIC alone in cases such as that described above.

IV. ANGULAR BIASING OF SCATTER

The twin techniques of splitting and Russian roulette used in MCBEND during the tracking of a particle depend upon splitting or rouletting a particle once it is in a given state. This state is described by the particle's position, energy, time and direction and has an associated importance (the extent of S/R depending upon the importances of the current and previous state). If the probability of a particle getting to a state is low, but the importance of the state (ie the likelihood of the particle scoring) is high, then it is sometimes not enough to split the particle once it has reached this important state, for very few particles would enter it. This is the case in streaming problems, where scatter into a small range of angles is required for the particles to travel, say, along a duct to the region of interest. It would be preferable to artificially increase the probability of scattering into that small range of angles, and so increase the particle population in the required region. This is the principle behind biased sampling, where the true probability of transfer from one state to another is modified by the importance of the states.

A. Biased sampling

Consider a particle with weight \( W \) in a particular state \( j \). The particle can transfer from state \( j \) to one of a number of other states \( k \), the probability for doing so being \( P(j-k) \). The expected weight entering state \( k \) is \( P(j-k)W \). The probability distribution may be altered by multiplying each probability by a value \( \Phi_k^* \). The resulting biased probability distribution will usually need to be normalised, so that
\[ P'(j-k) = \frac{P(j-k)\Phi_k^*}{\sum_k P(j-k)\Phi_k^*} \] (4)

To get the correct total weight of particles entering a state, each particle's weight must be altered to compensate for its altered probability, thus
\[ W' = W \frac{P(j-k)}{P'(j-k)} \] (5)

The optimum function to be used for \( \Phi_k^* \) is
\[ \Phi_k^* = \frac{\phi_k^*}{\phi_j^*} \] (6)

where \( \phi_k^* \) is the expected score in the detector of a particle entering state \( k \), ie its importance. The importances used for this type of biasing are therefore those of the current and future states, not those of the current and previous states. This is the essential difference between S/R and biased sampling. If the parameter \( S \) is defined as
\[ S = \sum_k P(j-k)\phi_k^* \] (7)

then
\[ P'(j-k) = \frac{P(j-k)\phi_k^*}{\phi_j^* S} \] (8)
If the values of $\phi^*$ are exact, $S$ is identically equal to unity because the importance of a particle entering a state is equal to its expected importance on leaving it. Thus, for example, if a particle is in state $j$ and after scattering is still in state $j$, ie $k = j$, then its weight will not change. In practice, approximate values are used for $\phi^*$, $S$ will not be exactly one, and there will be some spread of weights. However, if a particle is in a state $m$ with a weight

$$W = \frac{1}{\phi^*_m}$$  \hspace{1cm} (10)

then its weight will always be given by

$$W = \frac{1}{\phi^*_k}$$  \hspace{1cm} (11)

when it enters state $k$, as long as the expected number of particles leaving a state per particle entering is given by $S$. If $S$ is non-unity, this may be achieved by performing S/R on the particles as they change state. The result is that all particles entering a state, by whatever route they have taken through other states, will all have the same weight. This is consistent with the philosophy behind the conventional use of S/R in MCBEND.

B. Implementation in MCBEND

There are two main requirements for a capability for angular biasing, namely the ability to bias the scatter and the provision of importance information to be used in determining the extent of the biasing. The algorithm used for biasing the angle of scatter is similar to that used in the forced flight method and to a large extent can be described in the same terms. Rather than the particle (biased sampling is currently restricted to neutrons) undergoing scatter into a direction determined by the natural energy loss laws, its direction is chosen by random sampling from the angular importances $\Phi^*(r,E,\Omega')$, where the notation is consistent with Figure 4. The angular importances for the incident energy are used because the secondary energy is not known; however, this should not cause a significant loss in efficiency.

The weight change applied to the particle is given by

$$W' = W \frac{\phi^*_k}{\phi^*_m}$$  \hspace{1cm} (9)

The sampling from $\Phi^*$ expressed in equation 4 is reproduced by the above process, the direction of scatter being sampled from $\Phi^*$ because it is impractical to construct probability distribution functions which include both the angular importances and the angular distribution of scatter as the two angular distributions do not readily map onto each other. The process is equivalent to sampling the direction of scatter as if its angular distribution were isotropic, then folding in an extra factor in the particle weight to account for anisotropy.

The variation of the angular importances is discretised with respect to space (the splitting mesh), energy (same group scheme as used for S/R) and angle (as illustrated in Figure 5), with the extent of the angular bins being defined by lines of latitude and longitude.

C. Other aspects of angular biasing

Angular biasing of scatter is not used over all the system, as conventional S/R in space and energy is an adequate means of variance reduction in most regions of a system, and it is only near a void or within a material with a low cross-section that angular biasing will provide additional benefit. In other words, the variation of angular importance away from streaming paths is generally close to being isotropic, and does not need to be specified.
Angular importances are therefore not required for the whole system, but only for those regions where angular biasing is considered beneficial. Two S/R schemes therefore exist in the same system, with angular importances taking over from conventional ones in the appropriate regions, the former being used in the S/R process as well as for angular biasing. The transfer from one S/R scheme to the other is taken into account by normalising the values of angular importance for a mesh/energy group to the conventional importance.

When specifying a conventional importance map, it is usual to restrict the difference in importance between meshes to a factor two. This also applies to angular importances, but it has been found that these show large variations as the edge of the duct is approached. This is illustrated in Figure 6, which shows angular importances at four distances from a boundary for a detector offset in the void at some distance from the region for which the importances are shown. The most important direction is known to be nearly parallel to the duct wall, the polar angle being measured from the outward normal to the wall. (The calculation from which the figure is derived is described later.) The distances in the key are in terms of mean free paths into the duct wall.

![Angular importance diagram](image)

**Figure 6 - Variation of angular importances at the edge of a duct**

The angular importance at the duct wall shows a large peak just above the perpendicular to the outward normal, but this variation diminishes with depth into the wall, so that at a depth of about half a mean free path, there is little variation in the angular importance. To represent the angular importances accurately, the user would have to specify splitting meshes a tenth of a mean free path thick. This is likely to be impractical in many cases, and an option is available for using splitting meshes of normal size with the input variation of angular importance being applied on the side of the mesh which aligns with the wall of the duct, and an isotropic variation being set by the code on the opposite side. Angular importances inside the mesh are determined by linear interpolation.

The ideal way to calculate angular importances would be by performing an adjoint Monte Carlo calculation. However, it can be as time-consuming to perform an adjoint streaming calculation as one in forward mode, whereas it is desirable for the calculation of importances to take only a small fraction of time devoted to the calculation proper. MCBEND could therefore not be expected to produce angular importances for the whole system. As seen above, however, angular biasing is most important in regions close to the walls of a duct, and will be more so in the duct which contains the detector. It is therefore feasible to perform an adjoint MCBEND calculation placing the adjoint source at the detector position and scoring angular fluxes over the walls of the duct, using the splitting mesh to define the scoring regions. The adjoint fluxes can be written by the code in a form suitable for direct inclusion as angular importance data. As a simpler alternative to this technique, the user may provide estimated angular importances, basing them on knowledge of the penetration paths through the system being modelled.

The polar axis of the angular importances may be specified with respect to the axes of the MCBEND geometry, or alternatively directed towards a point in space, eg the centre of a detector. The former specification is applicable if a general set of angular importances is available over large parts of the system, the latter being used when angular importances are estimated by the user and a simple set are employed to direct particles towards the detector.

Particles which have been biased into the most important directions will have a relatively low weight, and so may be subject to extensive loss by roulette when they enter a mesh which does not use angular importances. The capability takes account of the situation where many of the particles which exit a mesh into the duct along which they are to stream would be killed in roulette. (This assumes that angular importances are not specified in the duct.) The few surviving particles would then be split as the importance increased along the duct to the region of interest, although this splitting is largely artificial as no particles in the beam will be lost while travelling in the void. It is more efficient not to perform S/R on a particle as it enters the duct, but to allow it to travel along the duct without further S/R until it reaches a region of solid
material. The importance of such a region is likely to be higher than the one the particle had left on entering the duct, and so the particle would have a smaller probability of being killed. S/R is therefore switched off in void regions of the system.

D. Test case

The example to be described was designed to be a geometrically simple test for the angular biasing capability. It consists of a two-legged duct in cylindrical geometry as illustrated in Figure 7. The duct is bounded by a black boundary condition, so that the only path from the monoenergetic point source, situated at the end of the short leg of the duct, to the detector at the end of the long leg of the duct is via the scatter body at the corner. The material in the scatter body has a mean free path of 10cm and particles have a 50/50 chance of being absorbed or undergoing isotropic scatter without a change of energy.

![Figure 7 - Test case for angular biasing of scatter](image)

The geometry was covered by a splitting mesh with axial splitting planes spaced 0.1 mfp apart in the scatter body. One radial splitting mesh covered the scatter body and no azimuthal variation was considered. Initially all values of importance were set to unity. The only variance reduction technique used was angular biasing of the source (an existing option in MCBEND) to eliminate wasteful sampling of particles not directed at the scatter body.

Although often impractical to achieve for more complicated systems, accurate importances for this simple case were derived by performing an adjoint calculation with the source positioned at the end of the long leg of the duct. This gave monoenergetic importances for this simple case, although MCBEND can perform multigroup adjoint calculations for more general applications. As well as scoring "conventional" fluxes throughout the system, angular fluxes on the surfaces of the splitting planes within the scatter body were scored in a number of polar bins, the polar axis being parallel to the z-axis of the system (the information in Figure 6 was taken from this calculation).

The forward calculation was then repeated using the results of the adjoint calculation to provide conventional and angular importances for the system. Angular biasing was only used at the two splitting meshes at the edge of the scattering material, the angular importance more than 0.2 mfp into the scattering material being almost isotropic. The same values of angular importance were used for both splitting meshes, these values being the angular fluxes scored at the boundary between the two meshes and thus acting as an average of the angular variation over this region. The use of angular importances to bias the angle of scatter resulted in an increase in efficiency of about a factor seventy over the initial calculation.

Such increases in efficiency cannot be expected for realistic problems, mainly because it is generally impractical to provide accurate values of angular importances in the space/energy/angle detail required. However, simple estimates of the angular importance based upon a knowledge of the geometry and penetration paths of the system being analysed have been shown to give useful, e.g. a factor two or three, increases in efficiency for cases such as streaming along the fuel channel of a gas reactor and along a PWR cavity. The capability obviously has some way to go before its full potential is realised, but development of angular biasing of scatter and its companion, the provision of angular importances, form part of an ongoing programme of MCBEND development.

V. SUMMARY

The three techniques described in this paper enable the user to provide efficient acceleration for the Monte Carlo method as used in the MCBEND code. The MAGIC capability, which involves solving the adjoint diffusion equation, produces values of importance which are effective for deep penetration calculations with minimal user intervention. The forced flight capability has given large increases in calculational efficiency for collimated systems, and angular biasing of scatter has shown promise as the way forward for the development of a general capability for the acceleration of streaming problems.

While MAGIC is based upon the automation of a well-established method of acceleration, the other two capabilities extend the range of calculations which can be performed efficiently with MCBEND. They answer the criticism of the Monte Carlo method that automated acceleration techniques are only useful for bulk penetration, and point towards future developments in acceleration techniques.
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