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1983 J. Phys. A: Math. Gen. 16 2827

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A solution of the neutron transport equation using spherical harmonics

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Received 16 September 1982, in final form 1 February 1983

Abstract. A solution of the neutron transport equation is obtained by expanding the flux $\Phi(\mathbf{r}, \mathbf{\Omega})$ at position \mathbf{r} in direction $\mathbf{\Omega}$ as a series of the form:

$$\Phi(\mathbf{r}, \mathbf{\Omega}) = \sum_{l=0}^N (2l+1) \sum_{m=0}^l P_l^m(\cos \theta) [\psi_{lm}(\mathbf{r}) \cos(m\phi) + \gamma_{lm}(\mathbf{r}) \sin(m\phi)]$$

where $P_l^m(\cos \theta)$ is the associated Legendre polynomial of order l , m with θ and ϕ the axial and azimuthal angles, respectively, of $\mathbf{\Omega}$. $\psi_{lm}(\mathbf{r})$ and $\gamma_{lm}(\mathbf{r})$ satisfy first-order differential equations and are determined by eliminating terms with odd l and then using finite-difference or finite-element techniques on the resulting second-order system. Complicated algebra is involved in deriving this latter set of relations and FORTRAN subroutines have been written to calculate the necessary coefficients and specify the relevant differentials.

1. Introduction

The solution of the transport equation using spherical harmonics is well known (Davison 1957, Weinberg and Wigner 1958, Clark and Hansen 1964). However, its implementation as an algorithm in a computer program was, until comparatively recently, thought to be too complicated for other than one-dimensional geometries (Henry 1975) or low-order approximations in higher dimensions (Gelbard 1968). Beginning in 1970, a re-appraisal of the method was undertaken, mainly because other approaches were encountering difficulties (Reed 1972). Also since diffusion theory, which is an adequate approximation for many applications, arises naturally from the spherical harmonics method, further consideration seemed merited.

The flux $\Phi(\mathbf{r}, \mathbf{\Omega})$ at location \mathbf{r} in the direction of unit vector $\mathbf{\Omega}$ is expressed as a series of the form:

$$\Phi(\mathbf{r}, \mathbf{\Omega}) = \sum_{l=1}^{\infty} (2l+1) \sum_{m=0}^l P_l^m(\cos \theta) [\psi_{lm}(\mathbf{r}) \cos(m\phi) + \gamma_{lm}(\mathbf{r}) \sin(m\phi)] \quad (1)$$

where θ and ϕ are the axial and azimuthal angles, respectively, of $\mathbf{\Omega}$. $P_l^m(\cos \theta)$ is the associated Legendre polynomial of order l , m and the expansion derives its name

from the fact that

$$P_l^m(\cos \theta) \begin{pmatrix} \cos(m\phi) \\ \sin(m\phi) \end{pmatrix}$$

form unnormalised spherical harmonics (Whittaker and Watson 1954). The series is terminated at some value $l = N$, usually odd, and the approximation denoted by PN .

Preliminary investigations in one dimension indicated that the first-order differential equations resulting for the unknown coefficients or moments, $\psi_{lm}(\mathbf{r})$ and $\gamma_{lm}(\mathbf{r})$, were most conveniently solved by eliminating terms with odd l to yield a second-order system for which many algorithms were known (Fletcher 1974).

Difficulties caused by the complexity of the equations in higher dimensions were surmounted by writing a small computer program to derive the second-order system (Fletcher 1976a) and currently the transport equation may be solved in most geometries of interest using either finite-difference or finite-element approximations (Fletcher 1980).

2. Equations

The mono-energetic transport equations may be written (Clark and Hansen 1964):

$$\mathbf{\Omega} \cdot \nabla \Phi(\mathbf{r}, \mathbf{\Omega}) + \sigma_t(\mathbf{r})\Phi(\mathbf{r}, \mathbf{\Omega}) = \int_{\Omega'} (\sigma_s(\mathbf{\Omega}', \mathbf{\Omega}, \mathbf{r}) + \nu\sigma_f(\mathbf{r})k^{-1})\Phi(\mathbf{r}, \mathbf{\Omega}') d\Omega' + S(\mathbf{r}, \mathbf{\Omega}) \quad (2)$$

where $\sigma_t(\mathbf{r})$ is the total cross section, $\sigma_s(\mathbf{\Omega}', \mathbf{\Omega}, \mathbf{r})$ the scatter from $\mathbf{\Omega}'$ to $\mathbf{\Omega}$, $\nu\sigma_f(\mathbf{r})$ the fission production term, assumed isotropic, and $S(\mathbf{r}, \mathbf{\Omega})$ any external source. For the case of no external source the arbitrary constant k must be adjusted to balance production and loss of neutrons in the system. Further conditions imposed on $\Phi(\mathbf{r}, \mathbf{\Omega})$ are that it is continuous everywhere and zero at external surfaces for inward directions of $\mathbf{\Omega}$. Equation (2) may also be taken as a convenient expression for the multi-group approximation. $\Phi(\mathbf{r}, \mathbf{\Omega})$ becomes a column vector of fluxes, one for each energy group, $\sigma_t(\mathbf{r})$ a diagonal matrix and $\sigma_s(\mathbf{\Omega}', \mathbf{\Omega}, \mathbf{r})$ and $\nu\sigma_f(\mathbf{r})$ partially or completely filled matrices depending upon the scatter and fission cross sections. Thus the ensuing discussion also applies to the multi-group case.

Equations for $\psi_{lm}(\mathbf{r})$ and $\gamma_{lm}(\mathbf{r})$ are derived by substituting equation (1) in equation (2) and transforming the $\mathbf{\Omega} \cdot \nabla$ terms back to spherical harmonics whose coefficients must then be separately zero because of the orthogonality of these functions. In performing this process use is made of recurrence relations satisfied by $P_l^m(\cos \theta)$ (Margenau and Murphy 1956).

Further, it is assumed that scatter is independent of the direction of incidence. Hence $\sigma_s(\mathbf{\Omega}', \mathbf{\Omega}, \mathbf{r})$ becomes a function of $\mathbf{\Omega}' \cdot \mathbf{\Omega}$ and may be expanded as the series of Legendre polynomials shown below.

$$\sigma_s(\mathbf{\Omega}', \mathbf{\Omega}, \mathbf{r}) = \frac{1}{4\pi} \sum_{l=0}^{\infty} (2l+1)\sigma^l(\mathbf{r})P_l(\mathbf{\Omega}' \cdot \mathbf{\Omega}). \quad (3)$$

The foregoing procedure yields a coordinate-dependent linked set of first-order differential equations for the moments $\psi_{lm}(\mathbf{r})$ and $\gamma_{lm}(\mathbf{r})$ (Fletcher 1976a).

As an example, for rectangular geometry with $\mathbf{r} = (x, y, z)$ then

$$\mathbf{\Omega} \cdot \nabla = \cos \theta \partial/\partial z + \sin \theta \cos \phi \partial/\partial x + \sin \theta \sin \phi \partial/\partial y \quad (4)$$

resulting in the expressions

$$\begin{aligned}
 &2(l+m+1)\frac{\partial\psi_{l+1m}}{\partial z} + 2(l-m)\frac{\partial\psi_{l-1m}}{\partial z} + \frac{\partial\psi_{l-1m-1}}{\partial x} \\
 &\quad - \frac{\partial\gamma_{l-1m-1}}{\partial y} - \frac{\partial\psi_{l+1m-1}}{\partial x} + \frac{\partial\gamma_{l+1m-1}}{\partial y} \\
 &\quad + (l+m+2)(l+m+1)\left(\frac{\partial\psi_{l+1m+1}}{\partial x} + \frac{\partial\gamma_{l+1m+1}}{\partial y}\right) \\
 &\quad - (l-m-1)(l-m)\left(\frac{\partial\psi_{l-1m+1}}{\partial x} + \frac{\partial\gamma_{l-1m+1}}{\partial y}\right) + 2(2l+1)\sigma_l\psi_{lm} = 2S_{lm} \quad (5)
 \end{aligned}$$

and

$$\begin{aligned}
 &2(l+m+1)\frac{\partial\psi_{l+1m}}{\partial z} + 2(l-m)\frac{\partial\psi_{l-1m}}{\partial z} + \frac{\partial\psi_{l-1m-1}}{\partial y} \\
 &\quad + \frac{\partial\gamma_{l-1m-1}}{\partial x} - \frac{\partial\psi_{l+1m-1}}{\partial y} - \frac{\partial\gamma_{l+1m-1}}{\partial x} \\
 &\quad + (l+m+2)(l+m+1)\left(-\frac{\partial\psi_{l+1m+1}}{\partial y} + \frac{\partial\gamma_{l+1m+1}}{\partial x}\right) \\
 &\quad - (l-m-1)(l-m) - \left(\frac{\partial\psi_{l-1m+1}}{\partial y} + \frac{\partial\gamma_{l-1m+1}}{\partial x}\right) + 2(2l+1)\sigma_l\psi_{lm} = 2S'_{lm}. \quad (6)
 \end{aligned}$$

Dependence on (x, y, z) is understood and $\sigma_l = \sigma_t(\mathbf{r}) - \sigma'(\mathbf{r}) - \nu\sigma_t(\mathbf{r})k^{-1}\delta_{l0}$ where δ_{ij} is unity if $i = j$ and zero otherwise. In the above equations for $m = 1$, coefficients of ψ_{l0} must be doubled because implied $P_l^{-1}(\cos \theta)$ terms are not used when substituting the recurrence relations. S'_{lm} and S_{lm} arise from the expansion of the source in a similar manner to the flux.

3. Boundary conditions

Because spherical harmonics are independent, continuity of $\Phi(\mathbf{r}, \mathbf{\Omega})$ implies a similar condition for $\psi_{lm}(\mathbf{r})$ and $\gamma_{lm}(\mathbf{r})$ across any material interfaces. On an external surface, zero incoming flux is approximated by setting

$$\int_{\mathbf{\Omega} \cdot \mathbf{n} \leq 0} \mathbf{\Omega} \cdot \mathbf{n} P_l^m(\cos \theta) \begin{pmatrix} \cos(m\phi) \\ \sin(m\phi) \end{pmatrix} \Phi(\mathbf{r}, \mathbf{\Omega}) d\Omega = 0 \quad (7)$$

for l even (Davison 1957) where \mathbf{n} is the outwardly directed normal. At reflected boundaries the normal derivative of the moment is zero if the spherical harmonic is even there, and the moment itself is zero in the odd case.

4. Method of solution

All the work to be described in this section has been incorporated over a number of years into the MARC computer code (Fletcher 1976b) and a program specification is given in the appendix.

As an illustration, the equations for XY geometry and $N = 3$ will be considered. Because there is no z dependence, only even functions of θ , i.e. $l + m$ even, occur and $\partial/\partial z$ terms are clearly zero. On eliminating odd l moments, assuming, for clarity, $\sigma_l = \sigma_1$ if $l \geq 1$ and an isotropic external source, there results

$$\frac{1}{3}\nabla^2\psi_{00} - \frac{1}{3}\nabla^2\psi_{20} + 2A\psi_{22} + 4B\gamma_{22} - \sigma_0\psi_{00} = -S - \nu\sigma_1 k^{-1}\psi_{00} \quad (8a)$$

$$-\frac{1}{3}\nabla^2\psi_{00} + \frac{25}{21}\nabla^2\psi_{20} - \frac{20}{7}A\psi_{22} - \frac{40}{7}B\gamma_{22} - 5\sigma_1\psi_{20} = 0 \quad (8b)$$

$$\frac{1}{3}A\psi_{00} - \frac{10}{21}A\psi_{20} + \frac{30}{7}\nabla^2\psi_{22} - 10\sigma_1\psi_{22} = 0 \quad (8c)$$

$$\frac{1}{3}B\psi_{00} - \frac{10}{21}B\psi_{20} + \frac{15}{7}\nabla^2\gamma_{22} - 5\sigma_1\gamma_{22} = 0 \quad (8d)$$

where

$$\nabla^2 = \frac{\partial}{\partial x} \frac{1}{\sigma_1} \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \frac{1}{\sigma_1} \frac{\partial}{\partial y} \quad A = \frac{\partial}{\partial x} \frac{1}{\sigma_1} \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \frac{1}{\sigma_1} \frac{\partial}{\partial y}$$

and

$$B = \frac{1}{2} \frac{\partial}{\partial x} \frac{1}{\sigma_1} \frac{\partial}{\partial y} + \frac{\partial}{\partial y} \frac{1}{\sigma_1} \frac{\partial}{\partial x}.$$

A finite-difference or a finite-element approximation may be used to solve the foregoing system, the advantage of the latter being the ability to deal conveniently with irregular shapes (Fletcher 1980).

Equations 8(a)–8(d) could be solved simultaneously for ψ_{00} to γ_{22} . However, to prevent N restricting problem size, each relation in the set is treated in turn as a diffusion type equation with a modified source. Thus (8a) is evaluated for ψ_{00} initially using a guess for other moments. (8b) yields ψ_{20} with the new values of ψ_{00} incorporated. This procedure calculates new ψ_{22} and γ_{22} from (8c) and (8d) respectively. The whole process is then iterated until changes in the moments between evaluations are less than desired accuracy criteria. For eigenvalue problems (zero external source) the normal fission source powering technique is utilised (Fletcher 1974).

In the multi-group case, moment equations for the highest energy group are solved once through followed by those for the next highest and so on down to the lowest, using latest values where possible to take advantage of the predominant downscatter. The general iteration then takes the form outlined for the one-group approximation.

If $N > 3$ in two dimensions or $N > 1$ in three dimensions, the second-order system is complicated and difficult to derive, as may be inferred from equations (5) and (6). However, the quantity of arithmetic involved is trivial in computer terms and a small program has been written to derive the coefficients and associated differential operators for the moments in each equation. Using this precalculation, the method outlined previously is then able to deal with approximations for arbitrary N and most geometries of interest.

It should be emphasised that the coding which produces the equations for solution provides, as well as coefficients, the moments and differentials involved and inputs the results to the solution algorithm without any involvement of the program user. To move from a P1 to a P7 approximation necessitates only the replacement of 1 by 7 in the problem data. N is usually odd because $N = 2j$ or $2j + 1$, with j any integer, results in the same number of equations for solution (Fletcher 1974) and hence the

higher more accurate value is used, the only limit being permitted calculation cost or running time.

As a first example, the problem displayed in figure 1 has been solved using MARC. Because there is no scatter, SN methods have difficulty in producing a solution (Reed 1972). Table 1 shows ψ_{00} (the scalar flux) 0.1 centimetres from BC for various N using a mesh-centred finite-difference representation on a uniform 0.2 cm grid. In table 2 and figure 2, ψ_{00} along AC for $N = 7$ is presented along with values from a finite-element calculation using the same mesh. The lack of scatter implies that the exact solution becomes an integral of exponential terms from the source region and results obtained in this manner are also given in table 1.

Table 1. Scalar flux (ψ_{00}) 0.1 centimetres from BC for various N . A and C are the locations given in figure 1.

Distance	Approximation				Exact
	P1	P3	P5	P7	
0.1	0.194 754E-2	0.253 217E-2	0.262 871E-2	0.259 878E-2	0.260 33E-2
0.3	0.191 495	0.250 070	0.259 490	0.256 526	0.256 91
0.5	0.185 138	0.243 893	0.252 860	0.249 955	0.250 25
0.7	0.175 990	0.234 917	0.243 233	0.240 414	0.240 83
0.9	0.164 490	0.223 480	0.230 962	0.228 249	0.228 63
1.1	0.151 179	0.210 019	0.216 494	0.213 894	0.214 38
1.3	0.136 657	0.195 048	0.200 393	0.197 913	0.198 58
1.5	0.121 536	0.179 120	0.183 358	0.181 045	0.181 80
1.7	0.106 397	0.162 762	0.165 960	0.163 855	0.164 60
1.9	0.917 421E-3	0.146 432	0.148 662	0.146 789	0.147 54
2.1	0.779 743	0.130 514	0.131 854	0.130 220	0.130 76
2.3	0.653 786	0.115 310	0.115 858	0.114 461	0.114 90
2.5	0.541 254	0.101 046	0.100 922	0.997 550E-3	0.100 07
2.7	0.442 803	0.878 739E-3	0.872 138E-3	0.862 666	0.865 23E-3
2.9	0.358 369	0.758 823	0.748 264	0.740 836	0.742 61
3.1	0.287 119	0.651 027	0.637 841	0.632 253	0.633 50
3.3	0.227 923	0.555 220	0.540 573	0.536 575	0.536 94
3.5	0.179 414	0.470 927	0.455 777	0.453 086	0.452 85
3.7	0.140 150	0.397 434	0.382 520	0.380 844	0.380 26
3.9	0.108 720	0.333 877	0.319 736	0.318 793	0.317 93

A second example is shown in figure 3 and this has been solved using a finite-element approximation with nodes at the points specified in the diagram.

Vacuum boundary conditions clearly correspond to replacing the surface with purely absorbing material extending to infinity and it is of interest to see at what rate the approximate condition of equation (7) and the use of an absorbing medium tend to the same result.

For practical purposes, 5 cm of absorber represents an infinite extent and this is added on the appropriate surfaces. ψ_{00} at A and B for various N is shown in table 3 and figure 4. It can be seen that the A values almost agree by P11 but roughly a 2% variation at B is still present for P13. The difference is unaffected by increasing the absorber thickness. However, it should be mentioned that this is a difficult problem and agreement would usually occur for smaller N .

Table 2. Scalar flux along AC for test problem 1 with $N = 7$.

Position	Finite difference	Finite element
A 0 0		0.568 331
0.1 0.1	0.564 856	
0.2 0.2		0.562 668
0.3 0.3	0.553 415	
0.4 0.4		0.544 784
0.5 0.5	0.527 844	
0.6 0.6		0.511 332
0.7 0.7	0.482 768	
0.8 0.8		0.453 374
0.9 0.9	0.405 869	
1.0 1.0		0.349 393
1.1 1.1	0.275 756	
1.2 1.2		0.166 535
1.3 1.3	0.909 675E-1	
1.4 1.4		0.652 485E-1
1.5 1.5	0.439 958E-1	
1.6 1.6		0.352 675E-1
1.7 1.7	0.262 964E-1	
1.8 1.8		0.218 533E-1
1.9 1.9	0.176 903E-1	
2.0 2.0		0.137 908E-1
2.1 2.1	0.108 713E-1	
2.2 2.2		0.885 426E-2
2.3 2.3	0.708 317E-2	
2.4 2.4		0.576 711E-2
2.5 2.5	0.465 516E-2	
2.6 2.6		0.380 459E-2
2.7 2.7	0.309 396E-2	
2.8 2.8		0.253 811E-2
2.9 2.9	0.207 663E-2	
3.0 3.0		0.170 979E-2
3.1 3.1	0.140 854E-2	
3.2 3.2		0.116 166E-2
3.3 3.3	0.963 972E-3	
3.4 3.4		0.795 199E-3
3.5 3.5	0.664 280E-3	
3.6 3.6		0.547 928E-3
3.7 3.7	0.461 349E-3	
3.8 3.8		0.379 668E-3
3.9 3.9	0.322 786E-3	
C 4.0 4.0		0.264 252E-3

5. Discussion

A difficulty with the method is the treatment of internal voids where, since $\sigma_l = 0$, a zero denominator results in equation (8). The usual approach is to use cross sections which are about 10^{-7} of normal magnitude and this procedure works satisfactorily. However, a more rigorous algorithm is desirable.

The MARC code, itself, is substantially complete apart from, possibly, a link to a mesh-generation package so that advantage of the flexibility of the finite-element approach may be made use of without too much tedious data input.

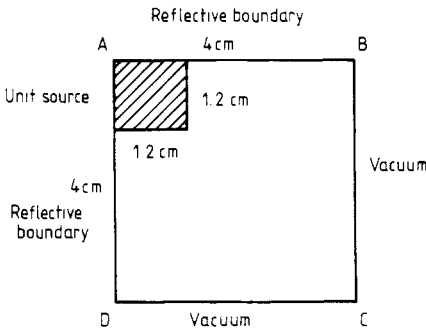


Figure 1. Transport theory test problem 1; $\sigma_t = 1$ and $\sigma_a = 0$.

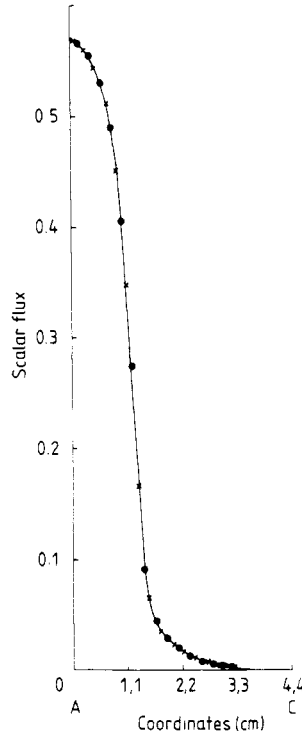


Figure 2. Scalar flux (ψ_{00}) along AC for test problem 1 with $N = 7$: x denotes the finite-element and ● the finite-difference technique.

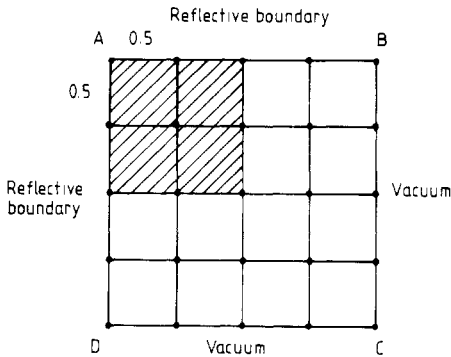


Figure 3. Test problem 2: for the unit source in the shaded region $\sigma_t = 0.75$, $\sigma_0 = 0.25$ and $\sigma_l = 0.75$ for $l > 0$.

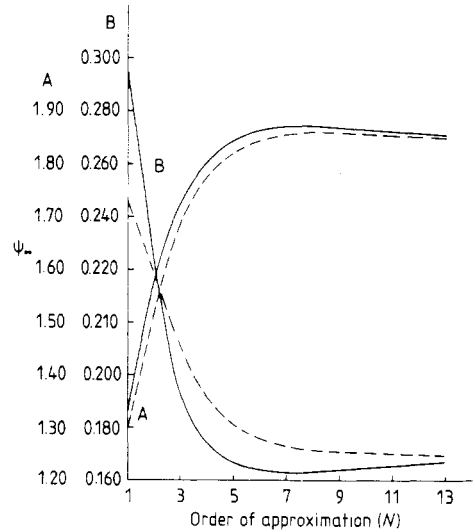


Figure 4. Dependence of the scalar flux on N at A and B for test problem 2. A comparison of boundary conditions is given; the full curve denotes the vacuum surface and the broken curve denotes the extended absorber.

Table 3. Variation with N of the scalar flux at A and B for test problem 2.

N	A		B	
	Vacuum	Added absorber	Vacuum	Added absorber
1	1.312	1.290	0.2924	0.2460
3	1.724	1.696	0.1944	0.2063
5	1.846	1.822	0.1669	0.1810
7	1.869	1.855	0.1634	0.1730
9	1.867	1.859	0.1643	0.1714
11	1.860	1.854	0.1656	0.1709
13	1.853	1.852	0.1666	0.1710

6. Conclusions

A solution of the multi-group transport equation using spherical harmonics has been successfully implemented as a computer code. Alternative finite-difference and finite-element representations are available, the latter enabling irregular meshes to be used.

Appendix. MARC

- (1) Name of code: MARC.
- (2) Computer: ICL2980, IBM3081.
- (3) Nature of physical problem solved: the multigroup, three-dimensional neutron transport and diffusion equations.
- (4) Method: the flux is expanded as a series of spherical harmonics. Odd-parity terms are eliminated from the resulting first-order equations for the coefficients of the series to yield a second-order system that is solved by a finite-element or finite-difference approximation.
- (5) Typical running times: cannot be specified since running time is dependent on the number of dimensions, mesh points or energy groups.
- (6) Unusual features: computer routines are used to derive the equations for solution.
- (7) Status: in use for production work.
- (8) References: Fletcher J K. A Users Guide to the MARC/PN Computer Code. TRG report 2911(R)1976. United Kingdom Atomic Energy Authority.
- (9) Machine requirements: problem dependent.
- (10) Material available: source code available from NEA Data Bank, 9119 Gif-sur-Yvette, Cedex, France, or RSIC, ORNL, PO Box X, Oak Ridge, Tennessee, USA.

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