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A three-dimensional method for calculating the hydraulic gradient in porous and cracked media

Hans Häggblom

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POSTADRESS: Kärnbränslesäkerhet, Fack. 102 40 Stockholm. Telefon 08-67 95 40

A THREE-DIMENSIONAL METHOD FOR CALCULATING THE HYDRAULIC GRADIENT IN POROUS AND CRACKED MEDIA

Hans Häggblom
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H Häggblom

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1. Introduction

When the water flow due to hydraulic gradients is calculated in two dimensions it is found that outlets into the ground surface are always obtained close to the bottom of a valley [1, 2]. This is not a real physical situation, because the valley would then be replaced by a lake. The drainage of the valley is of course due to a gradient in the perpendicular direction. This is an important reason for making three-dimensional calculations. Another reason is the ability to make realistic calculations of the dilution of migrating nuclides in a three-dimensional model. The obstacle for such a model is its complexity which may lead to long running times for computer programs with purely numerical solution methods. Much benifit can, however, be obtained from existing analytical two-dimensional solutions [2]. In this work it will be shown how such solutions can be used for synthezising three-dimensional solutions. It is expected that the method can be a base for a computer program with relatively short running times. The programming technique is also outlined.

2. The synthesis method

The differential equation for the piezometric head ψ in a porous medium with variable permeability K is [1, 2, 3]

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial \psi}{\partial x}\right)+ \frac{\partial}{\partial y}\left(K_y \frac{\partial \psi}{\partial y}\right)+ \frac{\partial}{\partial z}\left(K_z \frac{\partial \psi}{\partial z}\right) = 0 \tag{1}$$

By this formulation K is a tensor. Stokes [1] has shown that if K_x and K_y are constant, an equivalent isotropic formulation can be obtained by the transform

$$\xi = x\sqrt{\frac{K_z}{K_x}}$$

$$\eta = y\sqrt{\frac{K_z}{K_y}} \tag{2}$$

If the permeability is isotropic, constant in the x-direction and varying exponentially in the z-direction, and if furthermore ψ is independent of y, the transport equation can be written

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial z^2} + a\frac{\partial \psi}{\partial z} = 0 \tag{3}$$

where a is the exponential decay constant of K in the negative z-direction. This equation can be solved analytically [2]. It will now be shown how such solutions may be utilized for solving the corresponding 3-dimensional equation.

$$\nabla[K(z)\nabla\psi(x,y,z)] = 0 \tag{4}$$

For convenience, x, y and z will be replaced by $x_i, i = 1, 2, 3$. Consider a volume V within which a Lagrangian is defined by

$$L = \iiint_V \left[\sum_{i=1}^{3} \left(K \frac{\partial \psi}{\partial x_i} \right)^2 - \frac{\partial K}{\partial x_i} \psi \frac{\partial \psi}{\partial x_i} - \frac{1}{2} \frac{\partial^2 K}{\partial x_i^2} \psi^2 \right] dV \qquad (5)$$

An extremum value for L is obtained by the Euler equations:

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i} \left(\frac{\partial L}{\partial \psi_i} \right) - \frac{\partial L}{\partial \psi_i} = 0 \qquad (6)$$

where

$$\psi_i = \frac{\partial \psi}{\partial x_i} \qquad (7)$$

It is easily seen that application of Eq (6) upon the given Lagrangian leads to Eq (4). Thus, if an approximate solution ψ_p contains some parameters p_k and an extremum of the Lagrangian L is obtained by varying these parameters, this set of parameters gives the best approximation to the solution of Eq (4) that can be obtained from the set of functions ψ_p.

By partial integration of Eq (5) the Lagrangian can also be written in the following form:

$$L = \iint_S \left[K\psi \mathrm{grad}\psi - \frac{1}{2} \psi^2 \mathrm{grad}K \right] \bar{n} dS - \iiint_V \psi \nabla (K \nabla \psi) dV \qquad (8)$$

where S is the outer boundary of V and $\bar{n}$ is the outward-directed normal to this boundary. Then, if the ψ-function is replaced by an approximation which satisfies Eq (4)

the volume integral in Eq (8) will vanish. It should be observed that any solution of Eq (4) is convenient, independently of the boundary conditions. The utilization of this fact is the main difference between the synthesis method and the finite element method. In the latter one, arbitrary functions are chosen within a volume ΔV and the second integral in Eq (8) has to be calculated within this volume. The volume is limited by the limited ability of the chosen functions to fit the exact solution. In the synthesis method, the trial functions are solutions of the differential equation and can therefore be expected to fit the exact solution within a larger volume. The limiting factor is the ability to fit the boundary conditions.Because the volume integral in Eq (8) vanishes, the numerical work will be smaller in this method even with the same sizes of the partial volumes.

The trial functions may be chosen either as one set over the total volume (single-channel synthesis) or the volume can be divided into subvolumes with different function sets (multi-channel synthesis). For a three-dimensional problem it is customary to write the trial function as an expansion

$$\psi_p(x_1,x_2,x_3) = \sum_{n=1}^{N} \rho_n(x_1)\phi_n(x_2,x_3) \qquad (9)$$

where the functions ϕ_n are solutions of the corresponding two-dimensional differential equation and the coefficients ρ_n are solved so that ψ_p is the best possible approximation to the problem considered. For example, we can use solutions to Eq (3) for ρ_n and the expansion coefficients will then give the solution in the y-direction. It will be described how this method can be used for single-channel synthesis.

Another approach is to write the trial function as a combination of solutions in different directions

$$\psi_p(x_1,x_2,x_3) = \sum_{n=1}^{N} [a_n\phi_{1,n}(x_1,x_3)+b_n\phi_{2,n}(x_2,x_3)] \tag{10}$$

For the problem considered, this approach is more satisfactory in the sense that the coordinates x_1 and x_2 are handled on an equal basis. The functions $\phi_{1,n}$ and $\phi_{2,n}$ can then be solutions in the (x,z) and the (y,z) planes, respectively. It will be shown how this method can be used for multi-channel synthesis.

The two-dimensional functions considered will always be solutions of Eq (3). It is then convenient to return to the (x,y,z) notation for the coordinates. For the half-space with negative z-values, it is then assumed that the permeability is given by

$$K = K_o e^{az} \tag{11}$$

and that the maximum penetration depth is $-z_{max}$. It is then shown in ref 2 that a solution can be written in the form

$$\phi(x,z) = \frac{e^{-\frac{az}{2}}}{z_{max}} \sum_{n=1}^{\infty} f_n(x)\sin\left[\frac{\pi(n-\frac{1}{2})z}{z_{max}}\right] \tag{12}$$

where

$$f_n(x) = g \int_{-\infty}^{\infty} e^{\left[\frac{\pi(n-\frac{1}{2})\mu_n|\xi-x|}{|z_{max}|}\right]} h_1(\xi)\,d\xi \tag{13}$$

g is the acceleration of gravity.
$h_1(x)$ is the height of the groundwater surface along the x-axis. The constant μ_n is given by

$$\mu_n = \left\{1 + \left[\frac{az_{max}}{\pi(2n-1)}\right]^2\right\}^{\frac{1}{2}} \tag{14}$$

If N solutions of Eq (12) are obtained for different (x,y) planes, a three-dimensional solution can be obtained according to Eq (9). The coefficients $\rho_n(y)$ are obtained by replacing ψ in Eq (8) by ψ_p and seeking an extremum value of L with respect to ρ_n. In single-channel synthesis, the outer boundary is given by the total volume for the solution considered.

In Eq (12) the x-coordinate can of course be replaced by the y-coordinate. Then, consider a mesh structure in the (x,y) plane according to Fig 1. The lines y_m and x_m, where m and n are integers, define planes in the (x,z) and the (y,z) planes, respectively, for which the solutions $X_m(x,z)$ and $Y_n(y,z)$ are obtained. Further, consider a specific mesh defined by the lines $x_{n-1/2}$, $x_{n+1/2}$, $y_{m-1/2}$ and $y_{m+1/2}$. In a volume V_{mn} defined by this mesh and the z-planes $z=o$ and $z=-z_{max}$, an approximate solution to the problem considered is written as

$$\psi_p(x,y,z) = a_{m,n}X_m(x,z)+b_{m,n}Y_n(y,z) \tag{15}$$

The flow component in the x-direction is

$$J_x = K\frac{\partial\psi_p}{\partial x} = K\, a_{m,n}\frac{\partial X_m}{\partial x} \tag{16}$$

It is now required that this component is continuous over a vertical mesh boundary. The function X_m is a continuous function over any (y,z) plane. The permeability K is assumed to be discontinuous, but independent of x and y within the volume V_{mn}. Therefore, for preserving flow continuity,

$$K_{m,n}a_{m,n} = K_{m,n-1}a_{m,n-1} \tag{17}$$

Similarly, for continuity in the y-direction,

$$K_{m,n}b_{m,n} = K_{m-1,n}b_{m-1,n} \tag{18}$$

Because each partial volume has different expansion functions given by Eq (15), the approach is a form of multi-channel

synthesis. The coefficients $a_{m,n}$ and $b_{m,n}$ are discontinuous functions of the x- and y-coordinates. It should, however, be observed that

$a_{m,n} = a_{m,1}$ if K is independent of x

and

$b_{m,n} = b_{1,n}$ if K is independent of y.

3. The optimization procedure

Consider firstly the expansion according to Eq (9) with ϕ_n of the form given by Eq (12). The geometrical space will then be divided into subvolumes characterized by constant permeability. The Lagrangian will then equal the sum over the subvolumes of the surface integrals given by Eq (8). The continuity of flow is not preserved in this formulation and the surface integrals are then obtained as the arithmetic mean of the values on each side of the surface. In order to obtain the y-dependence of the coefficients ρ, they are assumed to be stepfunctions. Thus, the y-coordinate can be replaced by an index, k, which defines a micromesh within each subvolume. If the Lagrangian is minimized independently over each micromesh, a set of coupled equations is obtained. The number of equations equals the number of divisions in y-direction. The ρ-values can then be arbitrarily normalized if no additional constraint is put upon them. A suitable constraint is given by

$$\frac{1}{g}\iint_{S_{xy}} \psi(x,y,o)\,dxdy = \iint_{S_{xy}} h(x,y)\,dxdy \qquad (19)$$

where S_{xy} is the upper groundwater surface in the volume considered and $h(x,y)$ is the corresponding height. The l.h.s. of Eq (19) is then multiplied by a Lagrange multiplier, λ, and added to Eq (8). After optimization $\psi(x,y,z)$ is obtained as a function of λ and substituted into Eq (19). This gives the final solution.

Secondly, consider the expansion according to Eq (15). As an example, we assume that the map is divided into 3 meshes in the x-direction and 3 meshes in the y-direction (Fig 1). The two-dimensional calculations are performed along the lines x_1, x_2, x_3 and y_1 to y_3. Assume further that the permeability is equal to $K_{1,1}$ to the left of the line $x=x_2$ and equal to $K_{1,3}$ to the right of this line. Then

$$a_{m,2} = a_{m,1}$$

$$a_{m,3} = \frac{K_{m,1}}{K_{m,3}} a_{m,1}$$

$$b_{m,n} = b_{1,n}$$

It is sufficient to consider the first part of the Lagrangian given as

$$L_1 = \iint_S K\psi(\text{grad}\psi)\bar{n}ds \tag{20}$$

This part is obtained as

$$L_1 = \int_o^{z_{max}} dz \left\{ \sum_{k=1}^{3} \int_{y_{\ell-1/2}}^{y_{\ell+1/2}} dy \sum_{\ell=1}^{3} \left[F_{k,\ell}(x_{\ell+1/2},y,z) - F_{k,\ell}(x_{\ell-1/2},y,z) \right] + \right.$$

$$+ \left. \sum_{k=1}^{3} \int_{x_{k-1/2}}^{x_{k+1/2}} dx \sum_{\ell=1}^{3} \left[G_{k,\ell}(x,y_{k+1/2},z) - G_{k,\ell}(x,y_{k-1/2},z) \right] \right\} +$$

$$+ \sum_{k=1}^{3} \int_{x_{k-1/2}}^{x_{j+1/2}} dx \sum_{\ell=1}^{3} \int_{y_{\ell-1/2}}^{y_{\ell+1/2}} H_{k,\ell}(x,y,o)\,dy \tag{21}$$

where

$$F_{k,\ell} = \left[a_{k,\ell}X_k(x,z)+b_{k,\ell}Y_\ell(y,z)\right]K_\ell a_{k,\ell}\frac{\partial X_k}{\partial x} \tag{22}$$

$$G_{k,\ell} = \left[a_{k,\ell}X_k(x,z)+b_{k,\ell}Y_\ell(y,z)\right]K_\ell b_{k,\ell}\frac{\partial Y_\ell}{\partial y} \tag{23}$$

$$H_{k,\ell} = \left[a_{k,\ell}X_k(x,z)+b_{k,\ell}Y_\ell(y,z)\right]K_\ell\left(a_{k,\ell}\frac{\partial X_k}{\partial z} + b_{k,\ell}\frac{\partial Y_\ell}{\partial z}\right) \tag{24}$$

Because of the relationships between the coefficients with different k- and ℓ-values, the Lagrangian contains only 6 unknowns, namely, $a_{m,1}$, m=1 to 3 and $b_{1,n}$, n=1 to 3. Redundancy in the number of equations is avoided by summing up the integrals over partial volumes.

The function L_1 given by Eq (21) can then be written as a quadratic form in $a_{k,1}$ and $b_{1,\ell}$ given by

$$L_1 = \sum_{k=1}^{3}\sum_{\ell=1}^{3}\left(R_{k,\ell}a_{k,1}^2+S_{k,\ell}a_{k,1}b_{1,\ell}+T_{k,\ell}b_{1,\ell}^2\right) \tag{25}$$

where

$$R_{k,\ell} = \frac{K_{k,1}^2}{K_{k,\ell}}\left\{\int_0^{z_{max}}\left[\left(X_k\frac{\partial X_k}{\partial x}\right)_{x_{\ell+1/2}} - \left(X_k\frac{\partial X_k}{\partial x}\right)_{x_{\ell-1/2}}\right]dz + \right.$$

$$\left. + \int_{x_{k-1/2}}^{x_{k+1/2}}\left(X_k\frac{\partial X_k}{\partial z}\right)_{z=o}dx\right\}\left(y_{\ell+1/2}-y_{\ell-1/2}\right) \tag{26}$$

$$S_{k,\ell} = \frac{K_{k,1}K_{1,\ell}}{K_{k,\ell}} \left\{ \int_0^{z_{max}} dz \int_{y_{\ell-1/2}}^{y_{\ell+1/2}} \left[\left(\frac{\partial X_k}{\partial x} Y_\ell \right)_{x_{\ell+1/2}} - \left(\frac{\partial X_k}{\partial x} Y_\ell \right)_{x_{\ell-1/2}} \right] dy + \right.$$

$$+ \int_0^{z_{max}} dz \int_{x_{k-1/2}}^{x_{k+1/2}} \left[\left(X_k \frac{\partial Y_\ell}{\partial y} \right)_{y_{k+1/2}} - \left(X_k \frac{\partial Y_\ell}{\partial y} \right)_{y_{k-1/2}} \right] dx +$$

$$\left. + \int_{x_{k-1/2}}^{x_{k+1/2}} dx \int_{y_{\ell-1/2}}^{y_{\ell+1/2}} \left[\left(X_k \frac{\partial Y_\ell}{\partial z} \right)_{z=o} + \left(\frac{\partial X_k}{\partial z} Y_\ell \right)_{z=o} \right] dy \right\} \qquad (27)$$

$$T_{k,\ell} = \frac{K_{1,\ell}^2}{K_{k,\ell}} \left\{ \int_0^{z_{max}} \left[\left(Y_\ell \frac{\partial Y_\ell}{\partial y} \right)_{y_{k+1/2}} - \left(Y_\ell \frac{\partial Y_\ell}{\partial y} \right)_{y_{k-1/2}} \right] dz + \right.$$

$$\left. + \int_{y_{\ell-1/2}}^{y_{\ell+1/2}} \left(Y_\ell \frac{\partial Y_\ell}{\partial z} \right)_{z=o} dy \right\} \left(x_{k+1/2} - x_{k-1/2} \right) \qquad (28)$$

Eqs (25) to (28) are quite general, except for the number of meshes. A similar form can also be written for the rest of the Lagrangian. Finally, a Lagrange multiplier, λ, times the l.h.s. of Eq (19) can again be added to the Lagrangian and the coefficients are obtained by partial derivations, setting the results to zero, and again using Eq (19). This method seems simpler and more self-consistent than using trial functions depending only on x and z.

It should be noted that although the two-dimensional solutions are independent of the variation of the permeability in the x- and y-directions, the final solutions are not. Thus, the method is applicable for homogeneous media, for cracks and for large fissure zones imbedded in denser media.

4. Outlining a computer program

The proposed program HYGRA has a structure given in Fig 2. The main routine HYGRA reads a number of block names, except for the title and corresponding to different subroutines. The subroutine TOPOGRA is called for reading the topographic points defined by the height of the groundwater level in an arbitrary (x,y) mesh structure. MATRIAL reads material data in another arbitrary (x,y) mesh structure. PATHZON reads the starting points for different leakage paths. ADDIT reads some additional data, for example the number of points used for numerical integrations. EXECUTE is a control routine for the computations. MERGE combines the topographical and material meshes to a final mesh structure. MESH follows the flow from the start point to the outlet and determines the mesh at each time interval. MESHEAD calculates the piezometric heads and gradients in two-dimensional geometry within each mesh. MATRIX calculates the matrix elements given by Eqs (26) to (28), alternatively the matrix elements corresponding to expansion functions in (x,z) geometry only.

SYNCOFF calculates the synthesis coefficients, POINTFI calculates the final piezometric head in 4 points and corresponding gradient components. TRACE calculates the flow path for each time step. The results are listed in the subroutine LISTEDT.

The memory requirement is of course dependent upon the number of meshes. This, in turn, is dependent upon the topography and the ground heterogeneity. Thus, no conclusions can be drawn concerning this problem without extensive numerical experiments. Such tests must also be made for obtaining the necessary number of points in the numerical integrations. For keeping this number low, the integrations will be made by a Gaussian quadrature.

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Fig. 1

Mesh structure for multichannel-synthesis

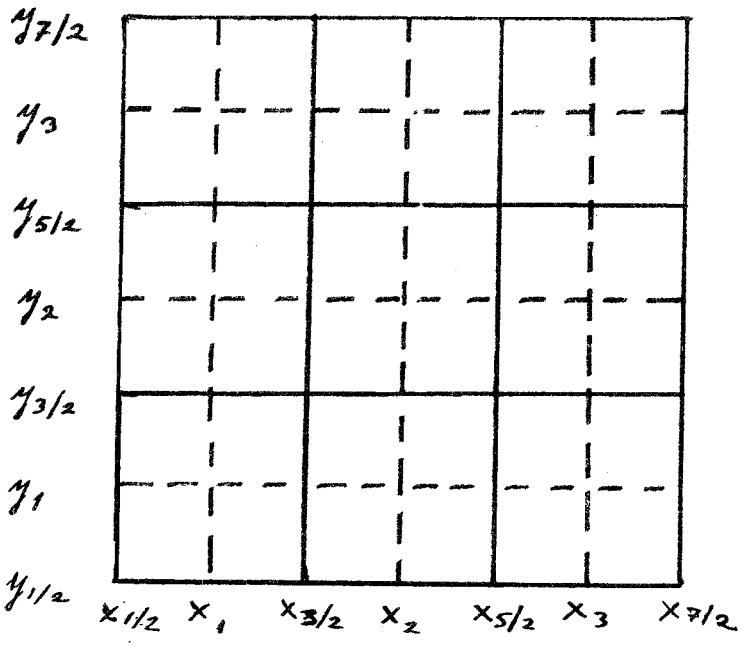
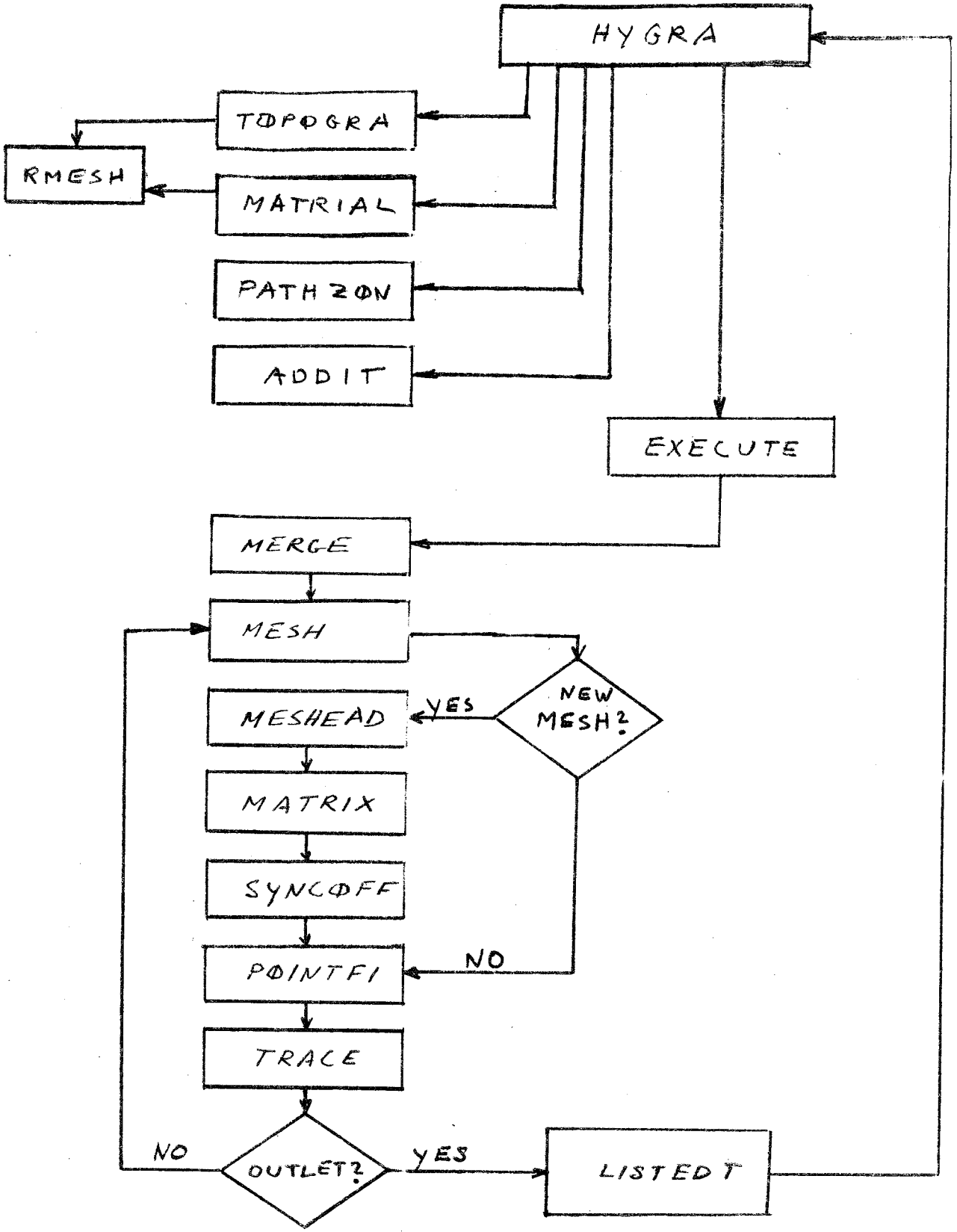


Fig. 2

Proposed structure of a computer program



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