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Numerical solution of field problems by nonconforming Taylor discretization

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An algorithm for the numerical solution of field problems is presented. The method is based on expanding the unknown function in a Taylor series about some nodal points so that the coefficients of the series for the various nodes are considered as unknowns. Discrepancy between the values resulting from Taylor expansions about distinct nodes is allowed if it is on the same order of magnitude as the estimated error resulting from the discretization. This enables considerable savings in computation effort in addition to the advantage of specifying the accuracy of the obtained solution. Geometrical flexibility, which enables handling complex boundaries for a large variety of field problems, is another advantage of the proposed scheme. The algorithm is applied to nonlinear steady-state heat-conduction. A test case is treated numerically, and for the evaluation of the scheme the results are compared with the analytical solution.

Keywords: numerical methods, partial differential equations, Taylor series, nonconforming expansions, nonlinear heat conduction

Introduction

Considerable effort is devoted to the development of numerical schemes for the solution of partial differential equations. The well-known and commonly used schemes are the finite element and finite difference methods. Each of these has its advantages and disadvantages, and especially in the field of heat and mass transfer, none is clearly preferred.¹ We believe that there is still room for new schemes and methods for numerical handling of such problems.

A new approach for manipulating approximations of k -times differentiable functions was proposed by Yomdin and Eliahai² using Kolmogorov's results^{3,4} concerning the optimal way to memorize a k -times differentiable function up to accuracy ϵ . They suggested that the approximation be represented by the coefficients of k -order Taylor expansions of the function about a collection of preselected nodal points. The distance between two neighboring points should be smaller than h with $h = O(\epsilon^{1/(k+1)})$.

Note that the scheme does not require that the expansions about distinct nodes coincide anywhere, and there is a discrepancy between the values that they assume (see *Figure 1*).

If this procedure is used to reconstruct a function that is known to be k -times differentiable, the discrepancy will not result errors greater than ϵ . However, if the procedure is used to approximate an unknown solution of a differential equation, the various Taylor expansions have to satisfy some "compatibility" conditions that will guarantee that they correspond to localization of a smooth function (in addition to the conditions offered by the differential equation itself). Following the guidelines of this general scheme, it is natural to require that the discrepancy be of the same order of magnitude as the error resulting from the Taylor approximation. Thus we do not spend unnecessary computational effort on fitting the local expansions with discrepancy smaller than the error that we expect for the given grid size and order of expansion. This feature of the new method is an attractive one in comparison with other existing methods.

In addition, this method offers excessive geometrical flexibility by allowing a user to choose the location of the nodal points and vary the distance between them. The number of neighboring nodes checked for continuity depends only on the order of the polynomial representing the dependent variable in the vicinity of

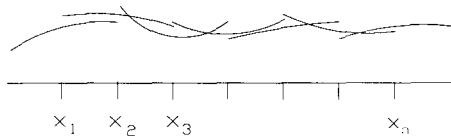


Figure 1. Schematic drawing of nonconforming discretization

each node. No other restrictions are present, and in principle the location and numbering order of neighboring nodes are not important. Moreover, as will be clarified in the next section, the computational effort is not influenced by the order of numbering of the nodes.

The proposed method has many potential applications beside the solution of partial differential equations. For example, Yomdin and Elihai developed an algorithm for global motion planning⁵ based on the same basic scheme. This and other currently developed algorithms are useful for computer-aided design and computer graphics.

The closest method to the one proposed here is the polynomial fitting. The difference is clear: polynomial fitting has been used until now only with accurate fitting as a method of obtaining the finite difference equation for each specific problem.⁶

The scope of the present work is the application of the method to numerical solution of engineering field problems. The scheme developed and presented is certainly not the only possible way to put the general ideas of Yomdin and Elihai into practical use. Further applications of the general ideas and other methods of putting it to work will be examined in forthcoming work. As a first application to field problems, nonlinear heat conduction was designated. A Fortran computer code was written, and a test case of heat conduction in a cylindrical rod of temperature-dependent conductivity was solved and compared with a known analytical solution.

The algorithm and application to nonlinear heat conduction

Steady-state heat conduction is presented by a Poisson equation with boundary conditions of imposed temperature or heat flux.⁷ With two independent variables, two types of boundary value problems may be considered, namely, the two-dimensional problem in cartesian coordinates

$$\frac{\partial}{\partial x} \left(k(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k(T) \frac{\partial T}{\partial y} \right) + \dot{q} = 0 \quad (1)$$

and the three-dimensional axisymmetric problem

$$\frac{1}{r} \frac{\partial}{\partial r} \left[k(T) \left(r \frac{\partial T}{\partial r} \right) \right] + \frac{\partial}{\partial y} \left(k(T) \frac{\partial T}{\partial y} \right) + \dot{q} = 0 \quad (2)$$

We consider the case in which the dependence of the conductivity on the temperature is given by

$$k(T) = k_s(1 + \alpha T) \quad (3)$$

and the heat source, \dot{q} , may be nonuniform, that is, may depend on the location (x , y , or r).

The concept behind the numerical method will be described using Figure 2, which shows an arbitrary distribution of points (shown as circles in Figure 2). Consider the point i_1 and five neighboring points i_2, \dots, i_6 , which outline the boundaries of a local region around it. The following polynomial function T_1 is the approximated, or discretized, temperature distribution in the vicinity of i_1 :

$$T(x, y)_1 = a_1 + b_1 x' + c_1 y' + d_1 x' y' + e_1 x'^2 + f_1 y'^2 \quad (4)$$

with

$$x' = x - x_1 \quad y' = y - y_1$$

Note that for simplicity, r in the axisymmetric representation will be represented by x . Two other such regions are shown in this figure to demonstrate the overlapping of regions. In this particular example a polynomial function of order 2 is chosen. For the neighborhood of any point i the coefficients a_i, \dots, f_i of the approximation T_i are unknown and yet to be determined. There are no restrictions on the relative position of the neighboring nodes; however, it is intuitively clear that they should be selected from the nearest vicinity of the central node. In particular, points on the boundary should be selected for nodes that are located near the boundary. Now the process of determining the unknown coefficients will be described. Substituting the polynomial function (4) into equations (1) and (2), differentiating, multiplying by $k(T)$ (T being represented by the polynomial), and finally setting x'_i and y'_i to zero (stating that the polynomial function satisfies the differential equation at the central point i) will result in the equation

$$\frac{I_c}{r} b + 2e + 2f = -\frac{\dot{q}}{k_s} - \alpha \left[b^2 + c^2 + 2a \left(e + f + \frac{I_c}{2r} b \right) \right] \quad (5)$$

with $I_c = 0$ for the planar case and $I_c = 1$ for an axisymmetric case. In the above equation the left-hand side contains the linear terms and the right-hand side the nonlinear terms, multiplied by α . Obviously, in

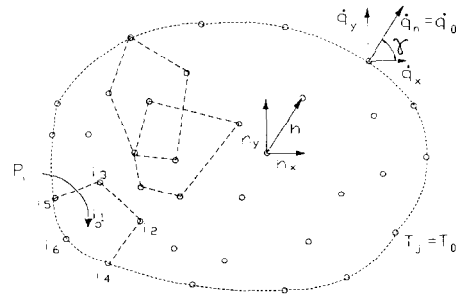


Figure 2. The discretization of the domain

case of constant conductivity ($\alpha = 0$) the nonlinearity vanishes. Equation (5), named hereafter the localized equation, is the only one in this algorithm that is unique to the present application. From now on, the description of the algorithm is generally applicable to any other field problem.

The above-mentioned localized equation provides

$$a_i + b_i h_x + c_i h_y + d_i h_x h_y + e_i h_x^2 + f_i h_y^2 = T_j \pm \epsilon \quad (7)$$

$$b_i \cos \gamma + c_i \sin \gamma + d_i (h_x \sin \gamma + h_y \cos \gamma) + e_i 2h_x \cos \gamma + f_i 2h_y \sin \gamma = -\frac{\dot{q}_j}{k(T_j)} \pm \epsilon' \quad (8)$$

where the permissible errors are

$$\epsilon = |\epsilon_0 h^3| \quad \epsilon' = \epsilon_0 h^2 \quad (9)$$

In equations (6)–(8), j is the index of any one of the neighboring nodes (such as i_2, \dots, i_6), i is the index of any central node (such as i_1), and h_x and h_y are the x - and y -components (respectively) of the relative position vector, h , between i and j (see *Figure 2*). The compatibility condition, equation (6), states that the expansion of T_i at the neighboring point j should approximately equal (within the permitted error) the value of T_j at point j , which is in fact the first coefficient of T_j , namely, a_j . The same idea leads to equations (7), stating that the expansion of T_i at a neighboring node j on the boundary should approximate the boundary prescribed temperature T_j . For neighboring nodes on a boundary with prescribed flux, equation (8) should be used. It is the result of adding the x - and y -components of discretized heat flux $\partial T_i / \partial x$ and $\partial T_i / \partial y$, respectively, and comparing them to the prescribed (normal to the boundary) flux (see *Figure 2*). The error permitted in the flux boundary condition is computed with an order of expansion that is 1 lower than the former continuity conditions, since the Taylor expansion was differentiated once.

The positive real number ϵ_0 in equation (9) is a constant used to evaluate the order of the permissible error according to the well-known relation for the truncation error $\epsilon = O(h^{n+1})$ (in our case the polynomial order n is equal to 2). One may take ϵ_0 as 1 initially. After the solution is completed, the error may be evaluated, as will be explained later, and a better estimation for ϵ_0 can be obtained.

In principle, having six equations for each nodal point and N nodes arbitrarily distributed in the domain (not counting the nodes on the boundary, which are used only for boundary conditions), one may write a $6N \times 6N$ global system of equations and solve it for the $6N$ unknown coefficients. Although possible, this would be a very ineffective way of solving the problem because of the size of the matrix obtained. A more effective way to solve the equation is to first treat separately each set of six equations obtained for each central node, in the following manner. The six equations may be written in matrix form as

$$[K] \cdot \{A\} = \{F\} \pm \{E\} \quad (10)$$

one out of six conditions needed at each point to determine the six unknown coefficients of its polynomial function. The other five conditions come from compatibility requirement

$$a_i + b_i h_x + c_i h_y + d_i h_x h_y + e_i h_x^2 + f_i h_y^2 - a_j = 0 \pm \epsilon \quad (6)$$

or from boundary conditions

where $[K]$ is of order 6×11 and $\{A\}$ is a column vector of dimension 11 that contains the six unknown polynomial coefficients of point i and the five a 's of the neighboring points. $\{F\}$ and $\{E\}$ are column vectors of dimension 6 containing the right-hand sides of conditions (5)–(8). Equation (10) is then segmented, dividing $\{A\}$ to $\{A_1\} = \{a_1, a_2, a_3, a_4, a_5, a_6\}$ and $\{A_2\} = \{b_1, c_1, d_1, e_1, f_1\}$, and so (10) breaks up into (11)–(12):

$$[K_{11}] \cdot \{A_1\} + [K_{12}] \cdot \{A_2\} = F_1 \quad (11)$$

which is the vector form of (5), and

$$[K_{21}] \cdot \{A_1\} + [K_{22}] \cdot \{A_2\} = \{F_2\} \pm \{E_2\} \quad (12)$$

which is the matrix form of the five compatibility or boundary conditions from (6)–(8). The set of six equations with eleven unknowns (10) can be replaced by one equation with six unknowns:

$$\begin{aligned} & [[K_{12}] \cdot [K_{22}]^{-1} \cdot [K_{21}] - [K_{11}]] \cdot \{A_1\} \\ & = [K_{12}] \cdot [K_{22}]^{-1} \cdot \{F_2\} - F_1 \\ & \pm [K_{12}] \cdot [K_{22}]^{-1} \cdot \{E_2\} \end{aligned} \quad (13)$$

This single row, expressing the relation between six a_1, \dots, a_6 coefficients for each nodal point, is substituted in a global matrix of the form (10), relating the a coefficients of all the points inside the domain. From the definition of the polynomial function (4) it is clear that the value of the unknown dependent variable at any point i is a_i . Hence, if in a linear case the values of T at the nodal points are needed only, the solution of global matrix equation (10) provides the complete solution of the problem. This solution is done by Gauss-Seidel iteration method with successive overrelaxation.⁶ The condition of the allowable error $\{E\}$ is fulfilled by allowing the respective error for each nodal relation (13) when solving the global matrix by iterations.

In a nonlinear problem, or in the case in which values of T between nodes are needed also, it is necessary to obtain the rest of the polynomial coefficients, b_i, \dots, f_i . This is done by writing the relations between each node to its neighbors (equations (6)–(8)) again, this time with the coefficients a known. Thus for each node a 5×5 matrix relation is obtained and solved separately. A nonlinear problem is solved by first assuming that $b_i, \dots, f_i = 0$; after a linear solution is

obtained, these coefficients are determined and are substituted into the right-hand side of (5). Then the whole process is performed iteratively until the successive values of coefficients a_i differ in less than E_i . Hence the nonlinear iterative procedure, as well as the whole solution, is performed until the local desired accuracy is achieved.

The procedure described above is very efficient for nonlinear problems, since the number of Gauss-Seidel iterations needed for the matrix solution decreases with the nonlinear iteration steps. This is achieved by using the solution of the last iteration as an initial guess for the following Gauss-Seidel solution. The same principle may be used when mesh density is concerned; it is possible to solve a problem with a coarse grid, finding by trial and error the appropriate ϵ_0 to be used in (9) and obtaining an approximate (but quick) solution. Then, better first-guess values may be used for a finer mesh for which the additional values for newly added points are interpolated from the coarse mesh solution. This procedure of refining the mesh may be automatically performed until the overall desired accuracy is obtained. The resulting discrepancy may be estimated by obtaining values for the solution at a node using the Taylor expansions about various neighboring nodes and comparing them. The solution is obtained with different values of ϵ_0 until the highest value, the one that does not increase the resulting discrepancy, is found. While this was done for a coarse mesh, it is appropriate to use the same value for finer meshes, ensuring optimal computer effort versus accuracy, where the effort is really important.

$$F(r) = \frac{q_0}{4} \left[w_0(R^2 - r^2) + \frac{w_1}{4}(R^4 - r^4) + \frac{w_2}{9}(R^6 - r^6) + \frac{w_3}{16}(R^8 - r^8) \right] \quad (17)$$

Computer codes that compute the exact and general numerical solutions were written. The numerical solution is performed in two different ways, namely, planar and axisymmetric modes, to verify the algorithm in both cases. Also, the use of regular and irregular meshes is demonstrated with these cases. The boundary conditions of the problem in the planar and axisymmetric cases are schematically shown in *Figure 3(a)* and *3(b)*, respectively. *Figure 4* shows the respective meshes

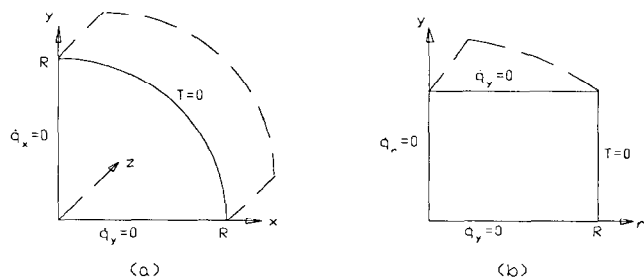


Figure 3. Boundary conditions of conduction in a cylindrical rod: (a) in a planar coordinate system and (b) in an axisymmetric coordinate system

One more important advantage is that the overall matrix solution is performed when the index numbers of the neighboring nodes are known for each node. Therefore a minimum-operation solution is always possible (in our case of five neighbors it is equivalent to a bandwidth of 6). The global numbering order of the nodes, or ordering of neighbours for each node, is of no importance. This is very important and effective in considering geometrical flexibility or using automatic mesh generation and refining.

A test case and results

A nonlinear conduction test case in cylindrical coordinates, as described by (2)–(3), is considered. The conductivity is temperature dependent, and heat generation, which depends on the radius, is expressed as

$$\dot{q}(r) = q_0(w_0 + w_1r + w_2r^2 + w_3r^3) \quad (14)$$

where q_0, w_i are constants. The boundary conditions for the problem are

$$\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0 \quad T|_{r=R} = 0 \quad (15)$$

The exact solution for this problem⁸ is

$$T(r) = \frac{-1 + \sqrt{1 + 2\alpha F(r)/K_s}}{\alpha} \quad (16)$$

where

plotted with lines connecting the central nodes to their preselected neighboring nodes. Of course, some of these lines represent connection in one direction, and some in two. This feature may be presented with different colors, but here only the general structure is demonstrated. Both meshes were generated by means of special-purpose mesh-generator codes, which were written for each case. An algorithm for a more general mesh generator should be the scope of another work, but no special difficulties are expected, considering

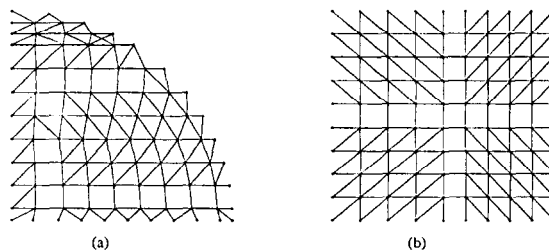


Figure 4. The computational meshes in (a) planar representation and (b) axisymmetric representation

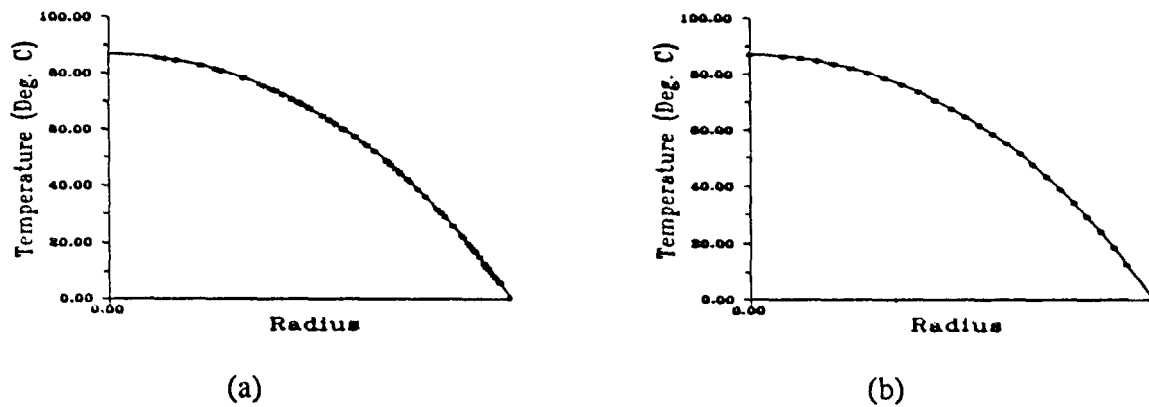


Figure 5. Numerical results (asterisks) compared to exact solution (solid curve) (a) in a planar coordinate system and (b) in an axisymmetric coordinate system

experience with similar mesh generators for finite element or finite difference use.

The results obtained are shown in *Figure 5(a)* and *5(b)* for the planar and axisymmetric approaches, respectively. The exact solution (16)–(17) is shown as a continuous curve; the numerical values of T are plotted as asterisks, according to their value r (distance from the origin in the planar case and from the left boundary in the axisymmetric one). As may be seen, even with the best resolution on screen, the numerical data fall exactly on the exact solution. If not so, scattered data should have been expected, since the r -distribution of both meshes (especially in the axisymmetric case) is not regular. For the shown meshes, the error was on the order of a hundredth of a percent, in comparison to the exact solution. The reduction of the error by using a finer mesh has been checked, too, resulting in the expected behavior according to (9). For the range checked, the value of ϵ_0 that gave optimal results for different mesh sizes remained constant.

Discussion

Our aim in this work was to present the principles of the nonconforming Taylor discretization method and to demonstrate its application in solving a particular problem in practice. Nevertheless, the advantages and disadvantages of the method in comparison with other numerical methods are of interest, and this discussion will briefly describe some of them. We feel that the following remarks and the attempt to compare the results with those obtained by the finite element method should be accepted with much care. They are based on preliminary and limited practice with the new scheme.

The proposed scheme has some features that we find attractive.

1. It is very easy to apply the scheme to new applications. Once one has the basic code that solves a certain PDE with the present algorithm, all that is needed to apply it to a different equation is to change the subroutine that contains the localized equations (5). (It is a matter of minutes to obtain the localized equations for a particular PDE such as (1)–(3)). The

application to a different PDE is a more tedious and longer process when done in the finite element or the finite difference method. Moreover, in comparison with the other methods mentioned, there is much less need for special knowledge and practice with numerical methods for such an application to be performed.

2. In solving the global equations an iterative method may be used. In this case we may wish to converge to the solution only within a known and finite error (which is related to the allowed discrepancy). This means that we do not attempt to converge to the solution of the set of equations to a better accuracy than the accuracy that we may expect for the given discretization. Therefore we may be able to save computer time and reduce round-off errors. This advantage depends on whether the matrix is of the kind that is solvable by iterative methods. In practice it worked for the examples presented in the preceding section, but determination of the conditions that ensure diagonal dominance will be the scope of further work.
3. Geometrical flexibility is another advantage of the suggested algorithm. Here, the flexibility of the input of the various nodes is even greater than the corresponding input in the finite element method. The reason is that the order of their numbering and connectivity to the neighbors has no impact on the validity and efficiency of the solution. However, one should bear in mind that no pre- and post-processors are available yet for the proposed scheme.

The finite difference method can be regarded as a special case of the proposed scheme. For example, the equations for central differencing are obtained in the present examples by choosing neighbors around the center point in a rectangular mesh and allowing no discrepancy. Choosing the neighbors in one preferred direction would lead to a forward differencing. It is therefore expected that one may face some of the problems occurring in the finite difference method and that some of the guidelines to overcoming them will apply here too. The above-mentioned advantages over finite differences have a price. It is the need for the computer

to repeat for each point the matrix manipulations (13) that are prepared, usually manually, to provide the algebraic finite difference equations. This disadvantage may be overcome by use of codes for symbolic manipulations that, it is hoped, can provide general equations that may be used readily. This feature of the algorithm may be regarded as a finite difference equation generator. Using only this feature, one loses the first advantage mentioned; however, it may well be that the time saved by the second advantage will compensate for these additional manipulations.

The objective of future works will be to prove and assess these and many other points. The authors feel that it is too early to make a thorough comparison at this stage. However, to give the reader a feeling for the efficiency of the algorithm, a comparison with the finite element method was performed. A finer grid for the former test case in an axisymmetric coordinate system was defined. To compare as fairly as possible the two methods, the order of interpolation and number of interpolation functions per typical length should be the same. Thus, for the present grid, 20×20 points were evenly distributed in the domain. With only 324 internal points, the global matrix to solve is also of rank 324. The nonlinear problem was solved in 87 seconds. The code was in Fortran with single-precision variables. For the finite element method a commercial code was used that runs in double precision. The domain was divided evenly into 20×20 eight-node elements, with a total of 1281 nodes. In this case this is also the number of degrees of freedom and the rank of global matrix. The solution time for the finite element method was 175 seconds on the same computer. The results obtained by nonconforming Taylor discretization were accurate to within 0.2% at the most, while for finite elements they were within 1% of accuracy only. The comparison is still not completely fair, since in the finite element model, internal heat load is defined uniformly on each element. The values entered were calculated at the center of the elements, which is probably the cause for the difference in results. However, this demonstrates a common situation in which the user is limited to the options available in a commercial code without being able to change them. Moreover, the comparison is also unfair because the finite element code is not necessarily as efficient and accurate as it would be if it were written especially to solve the specific equation rather than being a general-purpose code. Another difference is that the present code for noncon-

forming Taylor discretization does not necessarily use the most efficient solvers possible, and efficiency will probably be improved in future works. In general, considering feature 1 above and the comparatively efficient and accurate solution obtained, the comparison with the finite element method is encouraging.

Summary

A first implementation of the nonconforming Taylor discretization method to the solution of field problems was presented. It was applied to a nonlinear conduction problem, tested, and compared with the analytical solution. The results were very encouraging. The efficiency, simplicity, and flexibility of this scheme were demonstrated. The ability to estimate the error and to reduce computer effort for the solution were also demonstrated through the example. Further implementations for CFD and elasticity will probably be the scope of further works. Since the only part of the algorithm that deals with the specific application is that concerned with obtaining the localized equation (5), it is relatively easy to implement other applications once the code has been written. The authors feel that the great potential of the general idea of nonconforming Taylor approximations will develop in the future to many other applications and probably by different approaches.

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