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# The method of weighted residuals and its relation to certain variational principles for the analysis of transport processes

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**Abstract**—The approximation scheme entitled method of weighted residuals is extended to *systems* of differential equations and *vector* differential equations. The variational principles proposed by ROSEN, CHAMBERS and BIOT for unsteady-state heat transport are all shown to be applications of the method of weighted residuals. The von-Kármán–Pohlhausen method and the method of moments are also shown to be special cases. The method is illustrated by application to the problem of unsteady heat transfer to a fluid in ideal stagnation flow.

## INTRODUCTION

APPROXIMATE analytical solutions to partial differential equations are useful when exact analytical solutions are too difficult or impossible to obtain or when the work to find a numerical solution cannot be justified. For the heat transport equation, techniques have been developed by ROSEN [1], CHAMBERS [2] and BIOT [3, 4] to approximate the solution using some modification of the calculus of variations. It is shown below that these approximating techniques are all applications of the method of weighted residuals using the Galerkin criterion. An example shows how the method may be used to generate approximate solutions to transport problems arising in chemical engineering.

## METHOD OF WEIGHTED RESIDUALS

The application of the method of weighted residuals to solve a single scalar differential equation is discussed by CRANDALL [5] and KANTOROVICH and KRYLOV [6]. For analysis of transport phenomena, it is necessary to apply the method of weighted residuals (abbreviated MWR) to *systems* of differential equations and to *vector* differential equations, including realistic boundary conditions; this generalization is outlined below. BIEZENO and GRAMMEL [7] briefly mention a special case of the application of MWR to systems of equations.

### *General discussion*

Given the system of differential equations, boundary and initial conditions governing transport, the general approach is to assume a trial solution whose functional dependence on position is chosen, but which includes undetermined functions of time. These functions are found by requiring that the trial solution satisfy the differential equation approximately.

Consider, for example, the system of equations describing simple heat conduction or other scalar transport:

$$\rho C \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0 \tag{1}$$

$$\mathbf{q} + k \nabla T = 0 \tag{2}$$

in the domain $G$, for $t > 0$

$$\mathbf{n} \cdot \mathbf{q} - h(\mathbf{x}, t)[T - \chi(\mathbf{x})] = 0 \tag{3}$$

on $\Gamma$, the boundary of $G$, and

$$T(\mathbf{x}, 0) = \psi(\mathbf{x}) \tag{4}$$

for $\mathbf{x}$ in $G$, where $\chi$ and $\psi$ are the given boundary and initial data. It is physically reasonable to distinguish between the equation of change (1), which rests ultimately on general definitions of content and flux, and the constitutive relation (2), which must be supported by experimental determinations of actual behaviour of particular materials. The method of weighted residuals (MWR) will be used to approximate the solution to this problem.

Take trial solutions

$$\bar{T}(\mathbf{x}, t) = T_0(\mathbf{x}) + \sum_{i=1}^{N} a_i(t) T_i(\mathbf{x}) \tag{5}$$

$$\bar{\mathbf{q}}(\mathbf{x}, t) = \mathbf{q}_0(\mathbf{x}) + \sum_{i=1}^{M} b_i(t)\mathbf{q}_i(\mathbf{x}) \tag{6}$$

where the choices of $T_0$, $T_i$, $\mathbf{q}_0$, and $\mathbf{q}_i$ are arbitrary. Suppose, for illustrative purposes only, that the initial conditions (4) can be satisfied exactly by an appropriate choice of $a_i(0)$, and also that the $b_i(0)$ can be so chosen that

$$-k\nabla\psi = \mathbf{q}_0(\mathbf{x}) + \sum_{i=1}^{M} b_i(0)\mathbf{q}_i(\mathbf{x}) \tag{7}$$

The unknowns, $a_i$ and $b_i$ in equations (5) and (6), are determined by making the trial solution approximately satisfy the differential equations, (1) and (2), and the boundary conditions, (3). In this example, the choice $\mathbf{q}_i = -k\nabla T_i$, $N = M$, $a_i = b_i$ satisfies equation (2) exactly, but in general such a simplification is not possible.

Define the residuals

$$r \equiv \rho C \frac{\partial \bar{T}}{\partial t} + \nabla\cdot\bar{\mathbf{q}} \tag{8}$$

$$\mathbf{R} \equiv \bar{\mathbf{q}} + k\nabla\bar{T} \tag{9}$$

$$r_\Gamma \equiv \mathbf{n}\cdot\bar{\mathbf{q}} - h(\bar{T} - \chi) \tag{10}$$

These characterize the extent to which the pair of functions $\bar{T}$ and $\bar{\mathbf{q}}$ satisfy the differential equations and boundary conditions. As the number ($N$ and $M$) of functions ($T_i$ and $\mathbf{q}_i$) is increased in successive approximations, one expects the residuals to become smaller; the exact solution is obtained when the residuals are identically zero. As an approximation to this ideal, the weighted integrals of the residual are made zero:

$$\int_G S_i r dV = 0, \int_G \mathbf{p}_j\cdot\mathbf{R} dV = 0 \text{ and } \int_\Gamma S_{\Gamma k} r_\Gamma dS = S \tag{11}$$

where $S_i$, $\mathbf{p}_j$, and $S_{\Gamma k}$ are the weighting functions. If $\bar{T}$ and $\bar{\mathbf{q}}$ are the exact solutions, then equations (11) are satisfied regardless of the choice of the weighting functions. These can be chosen in some five different ways, and each choice corresponds to a different criterion in the MWR. Once this choice is made, equations (11) become a set of $N + M$ first-order ordinary differential equations in the $N + M$ unknowns $a_i$ and $b_i$. The solution to these equations is substituted into equations (5) and (6) to give the approximate solution to the problem.

*Method of collocation*

If one chooses $S_i = \delta(\mathbf{x}_i - \mathbf{x})$, the Dirac delta function, then the residual $r$ is zero at the points $\mathbf{x}_i$, and hence the differential equation (1) is satisfied exactly at these points. When treating vector equations and systems of equations, full generality can be achieved only by using a hypervector representation [8]. In order to simplify the presentation, two special cases will be noted here. Case (i) corresponds to making zero the component of the residual $\mathbf{R}$ in an arbitrary direction, $\mathbf{e}$, at the point $\mathbf{x}_j$:

$$\text{(i)} \qquad \mathbf{p}_j = \mathbf{e}\delta(\mathbf{x}_j - \mathbf{x}) \tag{12}$$

Case (ii) corresponds to making the residual $\mathbf{R}$ zero at the point $\mathbf{x}_j$:

$$\text{(ii)} \qquad \mathbf{p}_j = \mathbf{R}\delta(\mathbf{x}_j - \mathbf{x}) \tag{13}$$

Note that $\mathbf{R}\cdot\mathbf{R} = 0$ is equivalent to $\mathbf{R} = 0$, which specifies three times as many conditions as does $\mathbf{e}\cdot\mathbf{R} = 0$. The boundary residual can be handled in a similar way, but the total number of conditions in equations (11) cannot exceed the total number of unknowns, $M + N$.

*Subdomain method*

The differential equations are satisfied on the average in each of several subdomains if the weighting functions are chosen as follows:

$$S_j = \begin{cases} 1 & \mathbf{x} \text{ in } G_j \\ 0 & \mathbf{x} \text{ not in } G_j \end{cases} \tag{14}$$

where the $G_j$ are non-overlapping parts of $G$. For vector equations there is again a wide variety of choices of the weighting function $\mathbf{p}_j$. Special case (i) corresponds to annihilating the e-component of the vector residual on the average in the subdomains $H_j$:

$$\text{(i)} \qquad \mathbf{p}_j = \begin{cases} \mathbf{e} & \mathbf{x} \text{ in } H_j \\ 0 & \mathbf{x} \text{ not in } H_j \end{cases} \tag{15}$$

For case (ii):

$$\text{(ii)} \qquad \mathbf{p}_j = \begin{cases} \mathbf{e}_{(1)}, \mathbf{e}_{(2)} \text{ and } \mathbf{e}_{(3)}, \mathbf{x} \text{ in } H_j \\ 0 \quad \mathbf{x} \text{ not in } H_j \end{cases} \tag{16}$$

the vector residual is zero on the average in the

subdomains $H_j$, as long as the three vectors $\mathbf{e}_{(1)}, \mathbf{e}_{(2)}$ and $\mathbf{e}_{(3)}$ are linearly independent. It is not necessary that $H_j = G_j$, although such a choice of the two types of subdomains is possible. The boundary residual is handled in a similar way.

*Method of least squares*

The generalization of the method of least squares presents some difficulty. In the simple case of a single scalar equation with residual $r[a_i(t)]$, the weighting function is chosen to be $S_i = \partial r/\partial a_i$. If the $a_i$ were undetermined constants rather than functions of time, this choice of $S_i$ would correspond to minimizing the mean square residual, $J = \frac{1}{2}\int_G r^2 dV$, with respect to the $a_i$. When the $a_i$ are functions of time, this interpretation is no longer valid, because the $J$ is minimized with respect to $a_i$ while keeping the derivatives $\dot{a}_i$ fixed. If $J$ is to be a minimum for all time among all possible functions $a_i(t)$, then the $a_i(t)$ must satisfy

$$\frac{\partial J}{\partial a_i} = 0 \quad \text{and} \quad \frac{\partial J}{\partial \dot{a}_i} = 0, \; i = 1, \ldots, N \qquad (17)$$

These two sets of $N$ conditions will be incompatible in general, as the example in the Appendix shows. On the basis of these remarks, it can be concluded that the direct extension of the least squares criterion is of doubtful significance when the $a_i$ are functions of time rather than constants.

However, the original version of the least squares criterion can advantageously be applied to systems of equations. For example, in seeking the steady-state solution to equations (1) and (2) the $a_i$ and $b_i$ are indeed constants. If the component residuals are $r(a_i, b_i)$ and $\mathbf{R}(a_i, b_i)$ the total mean-square residual must be written

$$J \equiv \frac{1}{2}\int_G (\kappa_1 r^2 + \kappa_2 \mathbf{R}\cdot\mathbf{R}) dV \qquad (18)$$

with $\kappa_1$ and $\kappa_2$ suitably chosen positive constants. The constants, $a_i$ and $b_i$, are chosen to minimize $J$.

*Method of moments*

In this method the weighting functions are members of any complete set of functions. COURANT and HILBERT [9] give examples of complete sets of scalar-valued functions; examples of complete sets of vector-valued functions are provided by MORSE and FESHBACH [10]. For the one-dimensional case, a complete system is $(1, x, x^2, \cdots)$. The terms

$$\int r dx, \qquad \int r x dx, \qquad \int r x^2 dx, \ldots \qquad (19)$$

are then called the zero-th, first and second moments of the residual, $r$.

*Galerkin method*

In the Galerkin method the weighting functions $S_i$ and $\mathbf{p}_j$ are chosen to be the approximating functions $T_i$ and $\mathbf{q}_j$, respectively. Alternatively, the trial solution may take the general form

$$\bar{T}(\mathbf{x}, t) = \bar{T}(a_1, a_2, \ldots, a_N, \mathbf{x}, t) \qquad (20)$$

in which case the weighting functions would be $\partial\bar{T}/\partial a_i$. Another version results if one takes as weighting functions the exact or approximate solution to the adjoint equation (e.g. Ref. [11]). The Galerkin method is closely related to a variational principle if one exists for the problem, as has been shown in a few specific cases [12–14]. Further work is being done to elucidate this connexion.

If (i) the problem can be solved using separation of variables, (ii) the approximating functions are taken to be the eigenfunctions, and (iii) the Galerkin criterion of MWR is used, then the solution generated by MWR (as $N$ approaches infinity) is the exact solution as found using separation of variables. Of course, MWR is not restricted to time-dependent problems; it can be used to reduce the number of independent variables in any system of partial differential equations. The resulting system of equations is simpler (it may be sets of ordinary differential equations or algebraic equations), but its solution remains only an approximate solution to the original problem. The MWR can also be applied to non-linear problems, one of its most attractive features.

In applications of MWR it is important to know how accurate a given approximation is, and whether or not successive approximations converge to the exact solution. The first question is seldom treated in the literature; one hopes that the approximation is a good one when the successive approximations cease to differ appreciably as the number of

approximating functions increases. Convergence of the approximate solution to the exact solution has been proved in one case by GREEN [15], who treated the problem

$$\frac{\partial^2\phi}{\partial x^2} - \frac{\partial\phi}{\partial t} - \phi g = , \tag{21}$$

$$\phi(x, 0) = \phi(0, t) = \phi(\pi, t) = 0 \tag{22}$$

by using MWR with the Galerkin criterion. GREEN proves that the approximations for $\phi$, $\partial\phi/\partial x$ and $\partial\phi/\partial t$ converge uniformly [9] to their exact values. Furthermore, under special cases, GREEN gives an estimate of the error at any point. KANTOROVICH and KRYLOV [6] prove convergence of the Galerkin method for special cases in which a variational principle exists for the problem. In addition, they point out that the weighting functions must be members of a complete set of functions if convergence is to be assured.

## UNIFICATION OF PREVIOUS THEORIES

When using the calculus of variations [16] to generate approximate solutions to eigenvalue or boundary value problems, one tries to find the function $\phi$ which makes the integral

$$\Phi(\phi) = \int_{t_0}^{t_1}\int_G \cdots \int F\left(\phi, x_1, \ldots, t, \frac{\partial\phi}{\partial x_1}, \times \right.$$
$$\left. \times \ldots, \frac{\partial\phi}{\partial t}, \ldots\right) dx_1 \ldots dt \tag{23}$$

stationary, a minimum, or a maximum. The functional $\Phi$ is a real number: the integrations must extend over definite ranges of all the independent variables on which the function $\phi$ depends. In addition, $F$ depends on the partial derivatives with respect to the independent variables.† Consequently, whenever a "variational principle" is stated such that (i) the functional, $\Phi$, is a function of one of the independent variables, as $t$, and (ii) the functional, $F$, depends on derivatives with respect to that independent variable, then calling the principle a variational principle is not fully justified. Indeed, the so-called variational principles of ROSEN [1], CHAMBERS [2] and BIOT [3, 4] can now be interpreted as applications of the method of weighted residuals.

† If $F$ did not depend on any time derivatives, e.g. $\partial\phi/\partial t$, then the integration with respect to $t$ would not be performed; $\Phi(t)$ could be considered as a real number which depends on the parameter $t$; and the calculus of variations could be used to formulate and solve a variational principle for $\Phi$ at each value of $t$.

### *Analysis of* ROSEN'S "*Variational Principle*"

In order to approximate the solution to the unsteady-state heat conduction equation, ROSEN [1] defines the integral

$$I(t) = -\int_G \left[\tfrac{1}{2}k(\nabla T)^2 + \rho C T\frac{\partial T}{\partial t}\right] dV +$$
$$+ \int_\Gamma Tk\mathbf{n}\cdot\nabla T\, dS \tag{24}$$

His "restricted variational principle" states that $I$ is to be made stationary ($\delta I = 0$) with respect to arbitrary variations in temperature when the heat flux is given on $\Gamma$ and $\partial T/\partial t$ is given in $G$. ROSEN shows that under these conditions the temperature satisfies the Euler equation

$$\rho C\frac{\partial T}{\partial t} - \nabla\cdot(k\nabla T) = 0 \tag{25}$$

For calculational purposes, ROSEN suggests expanding the temperature in the series

$$T(\mathbf{x}, t) = \sum_{i=1}^{N} a_i(t)T_i(\mathbf{x}) \tag{26}$$

where the $T_i(\mathbf{x})$ are an orthonormal set of known functions which satisfy the boundary conditions, and the $a_i$ are determined by the "variational principle". ROSEN gives no details on how $\partial T/\partial t$ is kept fixed when $T$ is varied; this is equivalent to keeping $\dot{a}_i$ fixed while varying $a_i$. When $I$ is stationary, the equations which the $a_i$ must satisfy are derived by putting equation (26) into equation (24) and applying the "variational principle":

$$\sum_{i=1}^{N}\int_G [\rho C\dot{a}_i T_i - \nabla\cdot(ka_i\nabla T_i)]T_j dV = 0, j = 1, \ldots, N \tag{27}$$

It should be noted that if equation (26) is to satisfy the boundary conditions for all values of $a_i$, one must have $a_1 = 1$; $T_1$ must satisfy the condition $-k\mathbf{n}\cdot\nabla T_1 =$ the given heat flux on $\Gamma$; and $\mathbf{n}\cdot\nabla T_i$

$= 0$ on $\Gamma$ for $i > 1$. These considerations were not pointed out by ROSEN but are clearly revealed when the "variational principle" is viewed within the framework of MWR.

Equation (27) can also be derived using MWR. Take the same trial solution (26), with the restrictions noted above, and substitute it into equation (25) to form the residual. Apply the Galerkin criterion to get

$$\int_G T_j \left[ \rho C \sum_{i=1}^{N} \dot{a}_i T_i - \nabla \cdot \left( k \sum_{i=1}^{N} a_i \nabla T_i \right) \right] dV = 0 \quad (28)$$

which is equation (27). Thus the set of ordinary differential equations for the $a_i$ can be derived by either the "variational principle" or MWR with the Galerkin criterion. Since the integral $I$ is a function of time, it is more appropriate to view the technique as an application of MWR using the Galerkin criterion than as a variational principle.

*Analysis of* CHAMBERS' *"Variational Principle"*

CHAMBERS [2] has stated a "variational principle" which is similar to that of ROSEN, except that $\partial T/\partial t$ is varied during the variation and $T$ is held fixed instead of vice versa. CHAMBERS gives no details to show how this principle can be used, but if the temperature is expressed as in equation (26), then CHAMBERS' "variational principle" becomes an application of MWR. The proof is similar to that given above, and the details are omitted.

*Analysis of* BIOT'S *Theory*

In order to solve the heat transport equation (25) with the radiation boundary condition

$$-k\mathbf{n} \cdot \nabla T = h(T - \chi) \quad (29)$$

where $\chi$ and $h$ are known functions of boundary position and time, BIOT [3, 4] introduces a heat flow vector, $\mathbf{H}$, defined such that

$$\rho C T + \nabla \cdot \mathbf{H} = 0 \quad (30)$$

With this definition the differential equation (25) becomes, for constant $\rho$, $C$ and $k$

$$\nabla \cdot \left[ \frac{1}{k} \frac{\partial \mathbf{H}}{\partial t} + \nabla T \right] = 0 \quad (31)$$

Equation (31) will hold if

$$\frac{1}{k} \frac{\partial \mathbf{H}}{\partial t} + \nabla T = 0 \quad (32)$$

and then the boundary condition (29) is satisfied if

$$\frac{1}{h} \mathbf{n} \cdot \frac{\partial \mathbf{H}}{\partial t} + \chi - T = 0 \quad (33)$$

The problem can be summarized as solving equation (32) with the restriction (30) and the boundary condition (33). BIOT'S "variational principle" is

$$\delta \left( \frac{1}{2} \int_G \rho C T^2 dV \right) + \int_G \frac{1}{k} \frac{\partial \mathbf{H}}{\partial t} \cdot \delta \mathbf{H} dV + \int_\Gamma \left( \chi + \frac{1}{h} \mathbf{n} \cdot \frac{\partial \mathbf{H}}{\partial t} \right) \mathbf{n} \cdot \delta \mathbf{H} dS = 0 \quad (34)$$

He shows that if equation (34) is satisfied for arbitrary variations in $\mathbf{H}$, (arbitrary except that $\mathbf{H}$ must satisfy equation 30), then $\mathbf{H}$ and $T$ satisfy equations (32) and (33). Next, BIOT expands $\mathbf{H}$ in a series

$$\mathbf{H}(\mathbf{x}, t) = \sum_{i=1}^{N} q_i(t) \mathbf{H}_i(\mathbf{x}) \quad (35)$$

where the $\mathbf{H}_i$ are a chosen set of functions, and the "variational principle" determines the functions $q_i(t)$, which BIOT calls generalized co-ordinates. If the "variational principle" is used, it is found that the $N$ $q_i$'s must satisfy the equations

$$\int_G \mathbf{H}_i \cdot \left[ \nabla T + \frac{1}{k} \frac{\partial \mathbf{H}}{\partial t} \right] dV + \int_\Gamma \mathbf{n} \cdot \mathbf{H}_i \left[ \frac{1}{h} \mathbf{n} \cdot \frac{\partial \mathbf{H}}{\partial t} + \chi - T \right] dS = 0 \quad (36)$$

$$i = 1, \ldots, N$$

This set of equations can be rearranged to indicate the explicit dependence on $q_i$ and its time derivative $\dot{q}_i$:

$$\sum_{j=1}^{N} q_j \left[ \int_G \mathbf{H}_i \cdot \nabla T_j dV - \int_\Gamma \mathbf{n} \cdot \mathbf{H}_i T_j dS \right] + \sum_{j=1}^{N} \dot{q}_j \left[ \int_G \frac{1}{k} \mathbf{H}_i \cdot \mathbf{H}_j dV + \int_\Gamma \frac{1}{h} \mathbf{n} \cdot \mathbf{H}_i \mathbf{n} \cdot \mathbf{H}_j dS \right] = - \int \chi \mathbf{n} \cdot \mathbf{H}_i dS$$

$$i = 1, \ldots, N \quad (37)$$

Equations (37) are solved for the $q_i(t)$, and then equations (35) and (30) give the approximate solution.

When MWR is applied to the system of scalar and vector equations (30, 32, 33), the same set of equations (37) to determine $q_i$ results. To see this, substitute the trial solution (35) for $\mathbf{H}$ and equation (26) for $T$ into the equations (30, 32, 33) to form the residuals

$$r = \rho C \sum_{j=1}^{N} a_j T_j + \sum_{j=1}^{N} q_j \nabla \cdot \mathbf{H}_j \tag{38}$$

$$\mathbf{R} = \frac{1}{k} \sum_{j=1}^{N} \dot{q}_j \mathbf{H}_j + \sum_{j=1}^{N} a_j \nabla T_j \tag{39}$$

$$r_\Gamma = \frac{1}{h} \sum_{j=1}^{N} \dot{q}_j \mathbf{n} \cdot \mathbf{H}_j + \chi - \sum_{j=1}^{N} a_j T_j \tag{40}$$

If one chooses $a_j = q_j$, $\rho C T_j = -\nabla \cdot \mathbf{H}_j$, then $r \equiv 0$. Make this choice and apply the Galerkin criterion to the residuals $\mathbf{R}$ and $r_\Gamma$ with the weighting functions $\mathbf{H}_i$ and $\mathbf{n} \cdot \mathbf{H}_i$, respectively. The sum of the volume and surface weighted averages is just equation (37). Hence, the same results are achieved when one uses the Galerkin criterion of MWR as when one uses the "variational principle" of BIOT. Since the "functional" of BIOT depends on time (in fact equation (34) shows that no "functional" exists), it is more appropriate to regard the technique as a disguised application of MWR using Galerkin's criterion.

BIOT [3, 4] extends his treatment to include temperature-dependent properties and anisotropic solids. He also uses trial functions of the more general form

$$\mathbf{H} = \mathbf{H}(q_1(t), \ldots, q_N(t), \mathbf{x}, t) \tag{41}$$

All these modifications can be handled using MWR; in the latter case the weighting functions are $\partial \mathbf{H}/\partial q_i$.

NIGAM and AGRAWAL [17], and later BIOT [18], include in the above formalism the convection of heat with a known velocity field; i.e. the important convective term $\rho C \mathbf{u} \cdot \nabla T$ is included in equation (1). In the same way, GUPTA [19] develops a "variational principle" for heat transfer to a fluid in fully developed laminar flow in uniform channels. All these "variational principles" are equivalent to applications of MWR with the Galerkin criterion, just as in the examples described here.

## DISCUSSION

Several points are clarified by viewing the "variational principles" of ROSEN, BIOT and others as applications of MWR. First, MWR is more general than any of these principles that use the Galerkin criterion, which is only one of some five possible criteria in MWR. Furthermore, MWR can be applied to any system of differential equations whether or not a "variational principle" has been derived.

In ROSEN's analysis, the question of which approximating functions satisfy which boundary conditions was noted and answered above. BIOT states [3] that the energy equation is satisfied exactly in his method. The energy equation is split into two equations, (30) and (31), and this approach is analogous to distinguishing between the equation of change (1) and the heat-flux constitutive relation (2). If equation (32) is regarded as equivalent to the constitutive relation, then equation (30) must be called the energy equation. Then the solution satisfies the energy equation exactly and the constitutive relation approximately. It is a matter for numerical computation to determine whether a better approximation results from satisfying both equations only approximately, or whether an even better approximation results from solving the single scalar equation (25) approximately.

CITRON [20] claims that BIOT's "variational principle" is related to a least squares criterion and that this gives a means for judging the relative accuracy of several approximate solutions. The "variational principle" as stated by CITRON is not that of BIOT, but rather is an application of MWR using the least squares criterion, the interpretation of which is in doubt when $q_i = q_i(t)$, as in BIOT's scheme.

In the past, various special cases of MWR have been used in the chemical engineering literature under a number of aliases. The von-Kármán–Pohlhausen method of boundary layer theory [21] is an application of the method of moments using a single approximating function. For the simplest case of flow past a flat plate, a velocity profile is

assumed which contains an unknown boundary layer thickness $\delta(x)$. This velocity is substituted into the momentum equation, which is integrated over the domain $0 < y < \infty$. The result is an ordinary differential equation in $\delta(x)$ which is solved to give the velocity as a function of $x$ and $y$. In order that the approximation be a good one, conditions may be placed on the class of admissible velocity profiles [21]; this can also be done in any of the five alternatives of MWR. Successive approximations can be calculated by introducing more undetermined functions, in addition to $\delta(x)$, and by applying the method of moments. In such a case, higher moments of the momentum equation are made zero; the weighting functions are $1, y, y^2, \cdots$. This extension of the Von Kármán–Pohlhausen method was outlined in a particular case by FUJITA [22], and a similar procedure can be used for other boundary-layer type problems. Because the method of moments includes a procedure for improving the approximation, the Von Kármán–Pohlhausen method should be viewed as the first step in a procedure of successive approximations. The other four criteria of MWR can also be applied to the same problems; the Von Kármán–Pohlhausen method is just a particularly simple application of the method of weighted residuals.

An advantageous coupling of MWR and numerical finite difference methods has recently been used by KAPLAN and BEWICK [11] and KAPLAN and MARLOWE [23] to reduce the computer time necessary to solve nuclear reactor problems; the number of independent variables was reduced from four to two by the use of MWR.

## EXAMPLE

A convective transport problem is solved using MWR, and the results are compared to the exact solution in order to illustrate the application of MWR. The problem is to calculate the transient heat or mass transfer to a fluid in ideal stagnation flow towards a flat interface; this problem earlier resisted both exact and approximate solution [24]. The situation is depicted in Fig. 1. The energy equation, in dimensionless form, becomes

$$\frac{\partial T}{\partial t} + N_{\mathrm{Pe}}\mathbf{u}\cdot\nabla T = \nabla^2 T \tag{42}$$

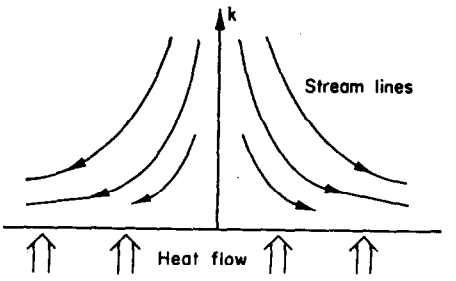


FIG. 1. Flow field.

with the initial and boundary conditions

$$\begin{aligned} T(\mathbf{x}, 0) &= 0 \\ T(z = 0, t) &= 1 \\ \lim_{z\to\infty} T(\mathbf{x}, t) &= 0, \end{aligned} \tag{43}$$

In the planar case the velocity is given by

$$\mathbf{u}' = a(x'\mathbf{i} - z'\mathbf{k})$$

or in dimensionless form

$$\mathbf{u} = 2(x\mathbf{i} - z\mathbf{k}) \tag{44}$$

Assume a trial solution of the form

$$\bar{T}(z, t) = \begin{cases} 1 + \sum_{i=1}^{N} a_i \left(\frac{z}{\delta_T}\right)^i & z < \delta_T(t) \\ 0 & z > \delta_T(t) \end{cases} \tag{45}$$

where $\delta_T(t)$ is a thermal boundary layer thickness, and the $a_i$ are constants. If

$$1 + \sum_{i=1}^{N} a_i = 0 \tag{46}$$

then equation (45) satisfies the boundary conditions, and if $\delta_T(0) = 0$ it also satisfies the initial conditions. The residual is formed by substituting equation (45) into equation (42); thereupon approximate solutions can be found by using four different criteria of MWR, as follows:

(i) Collocation: For the first approximation ($N = 2$), the residual is set equal to zero at the pair of points $z/\delta_T = \frac{1}{4}, \frac{3}{4}$. Owing to condition (46), when $N = 2$ only $\delta_T$ and one $a_i$ are free to be determined by the residual. The case $N = 1$ leads to the physically unrealistic solution $\delta_T(t) \equiv 0$. This choice ($N = 1$) can also be eliminated as a possible

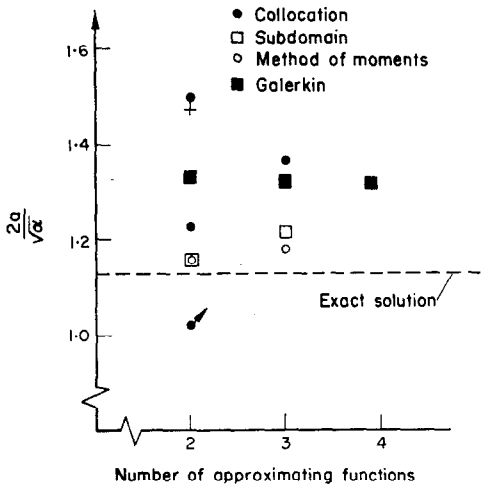


FIG. 2. Convergence of successive approximations.

trial function by noting that one term of the residual is then identically zero; this situation is to be avoided in the choice of trial functions. Two other first approximations correspond to setting the residual equal to zero at the pairs of points: $z/\delta_T = \frac{1}{4}, \frac{1}{2}$ or $\frac{1}{2}, \frac{3}{4}$ (♀ and ♂, respectively, in Fig. 2). For the second approximation, the points are taken as $z/\delta_T = \frac{1}{4}, \frac{1}{2}$ and $\frac{3}{4}$.

(ii) Subdomain: The domain $0 \leqslant z/\delta_T \leqslant 1$ is divided into $N$ equal parts. For $N = 3$, the subdomains become

$$0 \leqslant \frac{z}{\delta_T} \leqslant \frac{1}{3}, \quad \frac{1}{3} \leqslant \frac{z}{\delta_T} \leqslant \frac{2}{3}, \quad \frac{2}{3} \leqslant \frac{z}{\delta_T} \leqslant 1 \quad (47)$$

(iii) Method of Least Squares: This method is not used because $\delta_T$ is a function of time, a situation for which there is no direct extension of the method of least squares.

(iv) Method of Moments: The weighting functions are taken as $1, z/\delta_T, (z/\delta_T)^2, \cdots$.

(v) Galerkin: The weighting functions are taken as $\partial\overline{T}/\partial a_i$. If the residuals are formed according to the above prescription, one gets the set of differential equations

$$\frac{d\delta_T^2}{dt} + 4N_{\mathrm{Pe}}\delta_T^2 = \alpha_j \qquad j = 1, \ldots, N \quad (48)$$

where the $\alpha_j$ depend on the $a_i$. If this set of equations is consistent, one must have

$$\alpha_1 = \alpha_2 = \cdots = \alpha_N \equiv \alpha \quad (49)$$

Equations (49) and (46) determined the value of the constants, $a_i$, and this gives $\alpha$. Equation (48) is then solved for $\delta_T$:

$$\delta_T^2 = \frac{\alpha}{4N_{\mathrm{Pe}}}[1 - \exp(-4N_{\mathrm{Pe}}t)] \quad (50)$$

and this, combined with (45), constitutes the approximate solution to this problem. The dimensionless heat flux at the interface is then

$$N_{\mathrm{Nu}} = \frac{-2a_1}{\sqrt{\alpha}} N_{\mathrm{Pe}}^{1/2}[1 - \exp(-4N_{\mathrm{Pe}}t)]^{-1/2} \quad (51)$$

The value of $-2a_1/\sqrt{\alpha}$ is shown in Fig. 2 for the various methods and levels of approximation. Note that on the first approximation the spread of $-2a_1/\sqrt{\alpha}$ is 33 per cent of the largest value, but on the next approximation the spread decreases to 13 per cent of the largest value. The calculations become more difficult as $N$ increases, so not all the methods were carried through to the third approximation. All the methods seem to converge with increasing number of approximating functions, and there is no reason to doubt that they are converging to a common value (although it is not clear that they are converging to the exact solution recorded below). Such an observation justifies the engineer's confidence in the approximate solution when the mathematician is not yet able to provide rigorous assurances.

The exact solution to this problem has recently been found [25]:‡

$$T = \mathrm{erfc}\{zN_{\mathrm{Pe}}^{1/2}[1 - \exp(-4N_{\mathrm{Pe}}t)]^{-1/2}\} \quad (52)$$

The heat flux at the interface is then

$$N_{\mathrm{Nu}} = \frac{2}{\sqrt{\pi}} N_{\mathrm{Pe}}^{1/2}[1 - \exp(-4N_{\mathrm{Pe}}t)]^{-1/2} \quad (53)$$

The approximate and exact formulas for heat flux differ only in the value of the multiplicative constant, and the exact value of the constant is indicated on Fig. 2 for comparison. The approximate solution predicts exactly the functional dependence of $N_{Nu}$ on $N_{\mathrm{Pe}}$; this exact dependence cannot be assured in general.

‡ It should be emphasized that this exact solution was obtained *after* the approximate solutions described here were generated, and thus provided no insight into choice of trial functions.

## SUMMARY

It was shown that several "variational principles" for the unsteady-state heat conduction equation are in reality applications of the method of weighted residuals (MWR), and that greater clarity and more generality is achieved by viewing these principles within the framework of MWR. An example was worked to indicate the usefulness of several versions of the approximating method. Its utility will be improved as information about its convergence properties, systematic restriction of trial functions, and optimal weighting of component residuals becomes available. The method of weighted residuals holds promise as a general method for finding approximate solutions to transport problems in chemical engineering, particularly those with awkward constitutive relations, linear and nonlinear convective action, and complicated boundary conditions.


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## NOTATION

- $a$ Stagnation flow parameter (equation 44)
- $a_i$ Undetermined coefficients of $T_i$
- $b_i$ Undetermined coefficients of $\mathbf{q}_i$
- $C$ Heat capacity
- $D$ Thermal diffusivity, $k/(\rho C)$
- $\mathbf{e}_{(i)}$ Arbitrary vectors
- $\mathbf{f}$ Arbitrary function
- $F$ Arbitrary functional
- $g$ Arbitrary function
- $G$ Domain of integration
- $G_i$ $i$-th subdomain of $G$
- $h$ Heat transfer coefficient
- $H_j$ $j$-th subdomain of $G$
- $\mathbf{H}$ Heat flow vector
- $\mathbf{i}$ Unit vector in $x$-direction
- $I$ Variational integral
- $J$ Mean square residual
- $k$ Thermal conductivity
- $\mathbf{k}$ Unit vector in $z$-direction
- $L_0$ Characteristic length
- MWR (The) method of weighted residuals
- $N_{Pe}$ Peclet number, $L_0U_0/D - \frac{1}{2}aL_0^2/D$
- $N_{Nu}$ Nusselt number $= -\partial T/\partial z|_{z=0}$ (dimensionless)
- $\mathbf{n}$ Unit vector, normal to $\Gamma$ (positive outward)
- $\mathbf{p}_j$ Weighting function
- $\mathbf{q}$ Heat flux
- $q_i$ Generalized co-ordinates
- $r$ Residual
- $r_\Gamma$ Boundary residual
- $\mathbf{R}$ Residual
- $S$ Surface
- $S_i$ Weighting function
- $S_{Tk}$ Weighting function
- $T$ Temperature
- $t$ Time
- $\mathbf{u}$ Velocity
- $U_0$ Characteristic velocity
- $V$ Volume
- $\mathbf{x}$ Position vector $(x, y, z)$
- $\alpha$ Parameter used in equation (48)
- $\Gamma$ Boundary of $G$
- $\delta$ Variational symbol
- $\delta_T$ Thermal boundary layer thickness
- $\delta(\mathbf{x})$ Dirac delta function
- $\delta(x)$ Boundary layer thickness
- $\kappa_i$ Scale factors in $J$
- $\rho$ Density
- $\phi$ Arbitrary function
- $\Phi$ Functional of $\phi$
- $\chi$ Boundary values for temperature
- $\psi$ Initial distribution of temperature

Superscripts

- $-$ Trial solution
- $.$ Time differentiation
- $'$ Dimensional quantity

Subscripts

- $0$ First term in trial solution
- $i$ Approximating function

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## APPENDIX

Consider the problem

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0 \qquad 0<x<1,\quad 0<y<\infty$$

$$\phi(0,y)=\phi(1,y)=0 \qquad y>0$$

$$\left.\begin{aligned}\phi(x,0)&=x(1-x)\\ \phi(x,\infty)&=0\end{aligned}\right\} \qquad 0\leqslant x\leqslant 1$$

It is desired to show that the approximate solution generated by the method of least squares does not necessarily minimize the average square residual. Approximate $\phi$ by

$$\bar{\phi}=x(1-x)a_1(y)$$

$$a_1(0)=1 \qquad a_1(\infty)=0$$

The residual is

$$r=-2a_1+x(1-x)\ddot{a}_1$$

Apply the method of least squares to "minimize" $J$:

$$J=\int_0^1 r^2(x,y;a_1)dx$$

$$J=4a_1^2-\frac{2}{3}a_1\ddot{a}_1+\frac{1}{30}\ddot{a}_1^2$$

$$0=\frac{\partial J}{\partial a_1}=8a_1-\frac{2}{3}\ddot{a}_1 \qquad \frac{\partial J}{\partial \ddot{a}_1}=-\frac{2}{3}a_1+\frac{1}{15}\ddot{a}_1$$

Hence

$$a_1=\exp[-\sqrt{(12)}y]$$

and

$$J(a_1)=\frac{4}{5}\exp[-2\sqrt{(12)}y]$$

Let $b_1=\exp(-3y)$; then

$$J(b_1)=\frac{7}{10}\exp(-6y)$$

For $y<0{\cdot}14$, $J(b_1)<J(a_1)$, so the method of least squares does not minimize $J$ among all functions which satisfy the boundary conditions.

**Résumé**—La méthode d'approximation des résidus pesés est appliquée aux systèmes d'équations différentielles et aux équations différentielles vectorielles. Les principes variationnels proposés par Rosen, Chambers et Biot pour le transfert de chaleur non-stationnaire s'avèrent être des applications de cette méthode. La méthode de von Karman–Pohlhausen ainsi que la méthode des moments représentent également des cas spéciaux. La méthode est illustrée en l'appliquant au problème du transfert non stationnaire de chaleur entre un fluide et une surface plame.