Finite Elements in Fluids—Volume 2

Mathematical Foundations, Aerodynamics and Lubrication

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Chapter 1

Weighted Residual Methods and their Relation to Finite Element Methods in Flow Problems

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1.1 Introduction

Weighted residual methods are contrasted to finite elements methods for applications to flow problems. We first distinguish between principles which will generate the approximate solution and the choice of trial functions. For example, the Galerkin method is sometimes equivalent to the variational method, regardless of the choice of trial functions. The orthogonal collocation method is also seen to be equivalent to the Galerkin, and hence variational, method because the trial functions are orthogonal polynomials. This makes the orthogonal collocation method a discrete form of Galerkin's method in special cases. The importance of collocation-type methods is that quadratures need not be evaluated; several examples are given where this is advantageous.

The main difference between weighted residual methods and finite element methods is in the choice of trial functions or shape functions. Traditionally, weighted residual methods have used trial functions which are defined over the entire domain, whereas finite element methods have used shape functions defined over an element, with elements joined together to cover the entire domain. The various polynomials that have been applied to one-dimensional problems are described and their truncation errors listed. The method of orthogonal collocation on finite elements is then introduced by using as shape functions orthogonal polynomials on finite elements. This method has the advantage that quadratures need not be evaluated in non-linear problems. Conditions are given when it is equivalent to the Galerkin method and applications to time-dependent and two-dimensional problems are outlined. Finally the use of the residual allows for the automatic placement of elements, so that the elements are smallest in regions dictated by the solution. Such a scheme is not feasible in the finite element method when linear shape functions are used, since the residual is not defined.

To illustrate these features of the various methods, we consider applications to several flow problems. Entry-length calculations and boundary layer

flows characteristically have solutions with large gradients and the boundary layer flows often have singularities. These properties must be taken into account by efficient weighted residual methods while finite element techniques can be applied in a straightforward (though sometimes inefficient) manner. Flow through packed beds of spheres is shown to have an 8-fold symmetry which must be satisfied exactly for an efficient solution. Weighted residual methods can use trial functions obeying this symmetry, thereby achieving a $2^8 = 256$-fold reduction in the number of unknowns compared to finite element techniques. However, the trial functions utilizing this symmetry in weighted residual methods must be specially constructed for each problem. Applications in the field of petroleum reservoir analysis give useful insight into comparisons of different piecewise trial functions, as well as computing-time comparisons to finite difference methods. The non-linearities associated with the flow of non-Newtonian fluids add difficulties for efficient computing. In the finite element method, linear shape functions are especially convenient (because then the viscosity is constant over an element) but, for more accurate solutions, higher order polynomials have been used for Newtonian fluids. Such shape functions require recalculating the integrals in the finite element method each time the viscosity changes, as it does in each iteration for non-Newtonian fluids. Finally, flows with free boundaries utilize the convenient ability of finite element methods to handle diverse geometries.

1.2 Weighted residual principles

A variational principle is often used to generate the working equations in the finite element method. For a non-linear equation

$$\mathscr{D}(u(\mathbf{x})) = f(\mathbf{x})$$

application of the variational principle leads to the Euler equation of the form

$$\int_\Omega \delta u[\mathscr{D}(u(\mathbf{x})) - f(\mathbf{x})]\, d\Omega = 0 \tag{1.1}$$

Application of the variational method, for a trial function

$$u(\mathbf{x}) = \sum_{k=1}^{N} c_k u_k(\mathbf{x})$$

where the c_k are constants, gives

$$\int_\Omega u_j[\mathscr{D}(\textstyle\sum c_k u_k) - f(\mathbf{x})]\, d\Omega = 0 \tag{1.2}$$

The same equations arise from an application of the Galerkin method, when the residual, $N(\sum c_k u_k) - f$, is made orthogonal to the trial function, u_i. Thus there is always a Galerkin method which is equivalent to the variational method.

The variational method is usually applied without performing the integration by parts to obtain Equation 1.1 or 1.2. The trial function then need not be as continuous, since lower order derivatives appear. For example, the slow flow of a generalized Newtonian fluid through an irregularly shaped duct is governed by the variational principle (see Reference 1, p. 274)

$$\Pi(u) = \int_A \left[\int_0^{II} \eta(II')\, dII' + \mathbf{w} \cdot \mathbf{e}_{(z)} \frac{\partial p}{\partial z} \right] dA$$

$$II = d_{ij} d_{ij}$$

$$d_{ij} = \tfrac{1}{2}(w_{i,j} + w_{j,i})$$

where w_i is the ith component of velocity w, $w_{i,j} \equiv \partial w_i / \partial x_j$, and $\mathbf{e}_{(z)}$ is the unit vector in the $z(2)$ (or 3)-direction. The variation with respect to $\mathbf{w}$ yields

$$\delta\Pi = \int_A \left[2\delta w_{i,j} d_{ij} \eta(II) + \delta \mathbf{w} \cdot \mathbf{e}_{(z)} \frac{\partial p}{\partial z} \right] dA \tag{1.3}$$

while the Euler equation is from

$$\delta\Pi = \int_A \delta w_i \left[-2(d_{ij}\eta(II))_{,j} + \delta_{3i} \frac{\partial p}{\partial z} \right] dA + \int_{\Gamma_1} 2\eta(II)\, \delta w_i\, d_{ij} n_j\, d\Gamma \tag{1.4}$$

It is clear that the second derivative of w_i must exist if the trial functions are to be substituted into the Galerkin equation, Equation 1.4, since $2d_{ij,j} = w_{i,jj} + w_{j,ij}$, while in the variational formulation, Equation 1.3, only first derivatives of velocity appear. Furthermore, when the variational principle is a positive definite one, the equations resulting from Equation 1.3 will be symmetric and positive definite, thus leading to computational advantages. A further advantage of the variational principle is that natural boundary conditions are easily handled. The natural boundary conditions are contained in Equation 1.3 as $d_{ij} n_j = 0$ on Γ_1 while in the Galerkin formulation, the natural boundary conditions must be adroitly combined with the residual to obtain Equation 1.4 (see Reference 1, pp. 30, 150).

It is thus clear that a variational principle is useful, if one exists. The existence question is answered definitively using Fréchet derivatives as outlined in Reference 1, Chapter 9. Using that formalism, for example, we can prove that the steady state Navier–Stokes equations do not have a variational principle (Reference 1, Section 8.6) unless the inertial terms are zero or $\mathbf{w} \times (\nabla \times \mathbf{w}) = 0$. Thus, to include inertial terms we, of necessity,

must use the Galerkin method. We can, however, use the formulation as in Equation 1.3.

$$\delta\Pi = \int_A \left[2\delta w_{i,j} d_{ij} \eta(\mathrm{II}) + \delta w_i \rho w_j w_{i,j} + \delta \mathbf{w} \cdot \mathbf{e}_{(z)} \frac{\partial p}{\partial z} \right] \mathrm{d}A = 0 \qquad (1.5)$$

with the inertial terms added so as to obtain the correct Euler equation, as in Equation 1.4. Then, while the matrix arising in the finite element method will no longer be positive definite or symmetric, Equation 1.5 still only contains first derivatives, so that trial functions can be used which have no second derivative. Thus, even if the Galerkin method is applied, it is useful to understand variational principles. We note in passing that quasi-variational principles and the local potential method are also equivalent to the Galerkin method, and indeed these special constructs often obscure the mathematical basis for the approximate solution (see Reference 1, Chapter 10; Reference 2).

The orthogonal collocation method is an important method because of its relation to the Galerkin method and because of the extensions described below which combine it with finite element ideas. In a collocation method we set the residual to zero at a set of collocation points, e.g.

$$\mathscr{D}\left(\sum_{k=1}^{N} c_k N_k(\mathbf{x}) \right) - f(x)\Big|_{\mathbf{x}=\mathbf{x}_i} = 0 \qquad i = 1, \ldots, N \qquad (1.6)$$

and solve the resulting equations for c_k. In orthogonal collocation methods (Reference 3; Reference 1, Chapter 5) the trial functions are orthogonal polynomials. For illustrative purposes consider a one-dimensional problem, with $\mathscr{D}$ a second-order ordinary differential equation

$$\mathscr{D}\left(\frac{d^2u}{dx^2}, \frac{du}{dx}, u(x) \right) - f(x) = 0 \qquad 0 < x < 1 \qquad (1.7)$$

and appropriate boundary conditions at $x = 0$ and $x = 1$. The expansion function is taken as

$$u(x) = b + cx + x(1 - x) \sum_{i=1}^{N} a_i P_{i-1}(x) \qquad (1.8)$$

where $P_{i-1}(x)$ is an $(i - 1)$th order polynomial in x made orthogonal to all lower order polynomials using

$$\int_0^1 P_j(x) P_i(x)\, \mathrm{d}x = 0 \qquad i = 0, 1, \cdots, j - 1$$

Now it is clear that if the coefficients b, c, $\{a_i\}$ are known, the function $u(x)$ can be found for any x, since $P_{i-1}(x)$ are known functions. Conversely, if $u(x)$ is known at a set of $N + 2$ collocation points, then the coefficients

$b, c, \{a_i\}$ may be determined. The collocation points are taken as the N roots to $P_N(x) = 0$, which will be in $0 < x < 1$, and the end-points $x = 0, 1$. Derivatives of u, du/dx and d^2u/dx^2, can be written in terms of b, c, $\{a_i\}$, which are known in terms of $u(x_i)$, the function u at the collocation points. Thus it is possible to define the derivatives at the collocation points (Reference 1, p. 100)

$$u_i = u(x_i), \quad \left.\frac{du}{dx}\right|_{x_j} = \sum_{i=1}^{N+2} A_{ji}u_i, \quad \left.\frac{d^2u}{dx^2}\right|_{x_j} = \sum_{i=1}^{N+2} B_{ji}u_i \tag{1.9}$$

The orthogonal collocation method applied to Equation 1.7 then yields, similar to Equation 1.6,

$$\mathscr{D}\left(\sum_{i=1}^{N+2} B_{ji}u_i, \sum_{i=1}^{N+2} A_{ji}u_i, u_j, x_j\right) - f(x_j) = 0 \qquad j = 2, \ldots, N+1 \tag{1.10}$$

with two more equations for the boundary conditions at $x_1 = 0$ and $x_{N+2} = 1$. Now comes the important part. Because we have used orthogonal polynomials we can define a quadrature scheme

$$\int_0^1 f(x)\,dx = \sum_{i=1}^{N+2} W_i^{(N+2)} f(x_i) \tag{1.11}$$

which is exact when $f(x)$ is a polynomial of degree $2N + 1$ or less (Reference 1, p. 105). We can use this result to show that the collocation equations, Equation 1.10, are equivalent to the Galerkin equations for certain linear operators.

First assume the differential equation is of the form

$$(a_1 + a_2x)\frac{d^2u}{dx^2} + a_3\frac{du}{dx} - f(x) = 0 \tag{1.12}$$

with the boundary conditions $u(0) = a_4$, $u(1) = a_5$ and $f(x)$ an Nth order polynomial in x. The properties of the quadrature formula, Equation 1.11, can be used to show that the orthogonal collocation and Galerkin methods lead to identical results when the same orthogonal polynomials are used as trial functions in both methods (Reference 1, p. 135). If the problem is more general than Equation 1.12, i.e. the residual is not a polynomial or is a polynomial of degree greater than N, or is non-linear, then the exact correspondence fails. However, in those cases we can still say that the Galerkin method, using an approximate quadrature scheme, is equivalent to the orthogonal collocation method. It is the use of orthogonal polynomials, and the corresponding collocation points, that allows this result, and this is made particularly evident in the convergence results cited below.

Both variational and Galerkin methods require integration of the trial functions over the domain or finite elements. Such procedures are possible

a priori for certain types of non-linearities, like the $\rho \mathbf{u} \cdot \nabla \mathbf{u}$ term in Equation 1.5. However, other terms, like $\delta w_{i,j} d_{ij} \eta(\mathrm{II})$ in Equation 1.5, may be complicated enough to prohibit the integration at the start of the calculation, when no solution is known. Then the integrals must be recomputed throughout the iterative calculation and this increases the computation time drastically. The collocation method avoids this problem, because no integrals are evaluated, and the orthogonal collocation method is sometimes equivalent to the Galerkin method anyway. This advantage of the orthogonal collocation method is explored below.

In the subdomain method we use in place of Equation 1.2

$$\int_{\mathrm{Vol}_j} [\mathscr{D}(\sum c_k u_k) - f(\mathbf{x})] \, \mathrm{dVol} = 0,$$

thereby setting to zero the average residual in each subdomain Vol_j. Other methods are also possible by choosing other weighting functions in Equation 1.2 in place of u_j.[1,4]

1.3 Trial functions

In order to apply one of the methods of weighted residuals it is necessary to expand the unknown solution in a trial function. The analyst has a choice of two broad classes of trial functions. One class uses functions which are continuous and defined over the entire domain, while the other class divides the domain into subdomains or finite elements and uses trial functions defined only on the elements. The first class will be referred to here as global expansions, for ease in exposition.

The chief advantage of the global orthogonal collocation method is the very rapid convergence as the number of terms in the expansion is increased. For example, one study for an ordinary differential equation[5] found that the error was proportional to $(1/N)^{1.72N}$ where N was the number of collocation points. As N changes from 5 to 6, then, the error decreases by a factor of 100. By contrast, in a finite difference calculation of $O(\Delta x^2)$, where $N = 1/\Delta x$ is the number of grid points, a change of N from 5 to 6 leads to only 1·4 factor improvement in the error, or if the method is of $O(\Delta x^4)$ we get a 2·1 factor improvement. A theoretical study of global polynomial trial functions used with a variational principle showed that the error should decrease as $O(1/N)^{t-1}$ when the number of trial functions is increased (thus increasing the highest degree of polynomial considered).[6] In this expression $N + 1$ is the degree of polynomial and t is the continuity of the exact solution, and the proof requires $N + 1 \geq t$. In the example cited, faster convergence than this was found presumably because the trial functions were functions of x^2 and had certain symmetry properties already included. The rapid convergence of the global methods makes possible a reduction in the number

of collocation points, N, for a given accuracy and usually a marked reduction in computation time. However, the global expansions encounter difficulties when the solution has steep gradients in parts of the domain. In those situations a finite element type of approach is preferred, because elements can be bunched near the regions of steep gradients.

It is thus desirable to examine convergence results for piecewise polynomials to see what guidelines they give. The excellent paper by Ciarlet and coworkers[6] treats one-dimensional boundary value problems of the type

$$\sum_{j=0}^{n} (-1)^{j+1} D^j[p_j(x) D^j u(x)] = f(x, u(x)) \qquad 0 < x < 1$$

which have a corresponding variational principle. In addition to the convergence results for global polynomials, referred to above, they present results for various piecewise polynomials. The domain, $0 \leqslant x \leqslant 1$, is divided into a number of elements and a polynomial trial function is used on each element. The polynomials are listed in Table 1.1 together with the convergence results. We have a wide variety of choices available and the power, p, on the rate of convergence, expressed as $(1/M)^p$, depends on the degree of polynomial in the element. The more accurate methods have a higher p, necessitating a higher degree polynomial. The results of Ciarlet and coworkers[6] refer to variational methods whereas DeBoor and Swartz[7] use the collocation method on the subdivision of elements. They also show that the rate of convergence is increased in the collocation method on finite elements when the collocation points are Gaussian quadrature points rather than uniformly distributed. The Gaussian quadrature points correspond to the collocation points in orthogonal collocation on finite elements, as described below. The various choices of polynomials are compared in Table 1.2 depending on the degree of polynomial and the continuity of the trial function. Clearly there is overlap among the methods, even though the formulation and methods of solution are different.

Douglas and DuPont[8] treat time-dependent one-dimensional problems of the type

$$c(x, t, u)\frac{\partial u}{\partial t} = a(x, t, u)\frac{\partial^2 u}{\partial x^2} + b\left(x, t, u, \frac{\partial u}{\partial x}\right)$$

with a collocation method using cubic polynomials on each element. They, too, find that the rate of convergence is increased (to Δx^4) if the collocation points are the Gaussian quadrature points, whereas the convergence goes as Δx^2 for collocation points distributed uniformly on each element. Douglas[9] extends this work for linear problems when the polynomial is of degree $N + 1$. Gaussian quadrature points are used (i.e. orthogonal collocation on finite elements) to find that the convergence goes as Δx^{N+2} globally and Δx^{2N} at the collocation points.

Table 1.1 Comparison of properties of various piecewise polynomials*

Name	Degree of polynomial	Continuity of trial function†	Number of unknowns per element (after continuity)	Rate of convergence‡ as $M \to \infty$
Smooth Hermite§ $m = 1, 2, \ldots$	$2m - 1$	$m - 1$	m	$\left(\frac{1}{M}\right)^{2m-1}$
Non-smooth Hermite§ $m \geqslant 2k; k = 1, 2, \ldots$	$m - 1$	$k - 1$	$m - k$	$\left(\frac{1}{M}\right)^{2m-1}$
Spline functions§ $m = 2, 3, \ldots$	$2m - 1$	$2m - 2$	1	$\left(\frac{1}{M}\right)^{2m-2}$
Orthogonal collocation‖ on finite elements (second-order equations) $N = 1, 2, \ldots$	$N + 1$	1	N	at end of elements: $\left(\frac{1}{M}\right)^{2N}$ interior to elements: $\left(\frac{1}{M}\right)^{N+2}$

* Deduced from Reference 6§ and Reference 7‖; both for second-order ordinary differential equations.
† For example, if entry is t, then approximate solution $u \in \zeta^t$.
‡ t is the continuity of the exact solution; M is the number of subdomains.
§ Variational method.
‖ Orthogonal collocation method.

Table 1.2 Piecewise polynomials in one dimension

First entry is the degree of polynomial.
Second entry is the highest derivative of the solution which is continuous over the whole domain.

				Non-smooth Hermite			
Spline							
← 7	5	3	1	2	3	4	→
6	4	2	0	0	0	0	
Orthogonal collocation on finite elements		2	3	4	5	6	→
		1	1	1	1	1	
			5	6	7	8	→
			2	2	2	2	
			7	8	9	10	→
			3	3	3	3	
			↓ Smooth Hermite	↓	↓	↓	

1.4 Orthogonal collocation on finite elements in one dimension

Consider the ordinary differential equation, Equation 1.10, to be solved on $0 < x < 1$ together with boundary conditions at $x = 0, 1$. We divide the domain $0 < x < 1$ into NE elements by placing the dividing points at x_l, $l = 1, \ldots, NE + 1$, with $x_1 = 0$ and $x_{NE+1} = 1$. Within each element we define a new variable $s^l = (x - x_l)/\Delta x_l$, $\Delta x_l = x_{l+1} - x_l$, and place interior collocation points at the roots to $P_N(s) = 0$, where P_N is a shifted Legendre polynomial defined on $0 \leqslant s \leqslant 1$. Within each element the variable s^l goes from zero to one. Applying the usual procedure of orthogonal collocation[1] we write the differential equation at the interior collocation points in terms of the value of the solution at the collocation points in the same element. Thus we get

$$\mathscr{D}\left(\frac{1}{\Delta x_l^2}\sum_{i=1}^{N+2} B_{ji}u_i, \frac{1}{\Delta x_l}\sum_{i=1}^{N+2} A_{ji}u_i^l, u_j^l, x_l + s_j^l\Delta x_l\right) - f(x + s_j^l\Delta x_l) = 0 \tag{1.15}$$

$$j = 2, \ldots, N + 1; l = 1, \ldots, NE$$

where the matrices B and A are the same ones arising in Equation 1.10. At the division between elements we require continuity of the first derivative.

$$\Delta x_{l+1}\sum_{i=1}^{N+2} A_{N+2,i}u_i^l - \Delta x_l\sum_{i=1}^{N+2} A_{1i}u_i^{l+1} = 0$$

Two additional equations are written for the boundary conditions. For use on a computer we line up the variables u_i^l as one long vector u_k by defining $u_k = u_{(N+1)(l-1)+j}$, where l goes from 1 to NE and j goes from 1 to $N+1$, except for $l = NE$ when j goes to $N+2$ to get $u_{(N+1)NE+1} = u(x=1)$. If the problem is linear we can then write the set of equations as

$$\mathbf{AAu} = \mathbf{F} \tag{1.16}$$

and the matrix **AA** has the block diagonal structure shown in Figure 1.1.

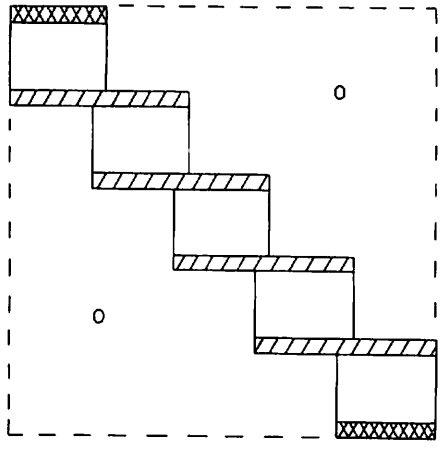

Figure 1.1 Matrix arising in method of orthogonal collocation on finite elements. The only non-zero entries are inside the solid blocks. The cross-hatched areas come from boundary conditions, the slashed areas come from continuity of the first derivative at the element boundaries and the other areas come from the differential equation

There is only one element of overlap, so that we need store only the blocks along the diagonal, as a three-dimensional array $AA(l, i, j)$ with $l = 1, \ldots, NE$ and $AA(l, N+2, N+2) = AA(l+1, 1, 1)$. Such matrices can be inverted using an efficient LU decomposition routine written by Graham Carey of the University of Washington, and the result can be stored on top of AA, in the same block diagonal structure. If the problem is non-linear a simple approach is to collect all the non-linear terms in **F** in Equation 1.16 and solve the equations iteratively, $\mathbf{AAu}^{k+1} = \mathbf{F}^k$. If **AA** is fixed (independent of k) the LU decomposition is carried out only once, and the iterations are performed with fore-and-aft sweeps, thus saving computation time. If this iteration scheme is not convergent then Newton-Raphson can be applied to obtain linear equations of the form Equation 1.16, and the matrix **AA** is inverted at each iteration.

As mentioned above, DeBoor and Swartz[7] have shown that for second-order equations the rate of convergence of the solution and first derivative

at the end-points of each element, $s^l = 0$ or 1, goes as Δx^{2N}, where Δx is the uniform element size, while the error decreases as Δx^{N+2} as $\Delta x \to 0$ for the solution at the interior collocation points. It is clear that this scheme can lead to very high order rates of convergence and, indeed, computations bear this out. Of course, as in any finite element method, the element sizes need not be uniform.

Once the calculation is completed, the residual can also be computed. As in any weighted residual method, the residual is the differential equation, evaluated for the approximate solution. It is zero at the interior collocation points of each element, since the solution was found by solving Equation 1.15. In between the collocation points, however, it is non-zero. Calculations have shown that as the approximate solution is refined the residual approaches zero at more and more points and the mean-squared residual also approaches zero (see, for example, Reference 5). Sometimes an upper bound on the error in the solution can be found as a function of the mean-squared residual, even when no exact solution is available.[5] Thus we want the residual to be small, and for the exact solution it is zero. After an orthogonal collocation solution is found on finite elements we can examine the residual. This is most easily done at the end-point of each element, although the interpolation polynomial can be used to find the solution, and hence the residual, anywhere in the domain. Additional elements can then be added in places where the residual is large and the calculation is repeated. In this way we end up with the elements in exactly the place they are needed. Application of this idea to a chemical engineering problem led to very rapid convergence as well as different element sizes whose ratio was as high as 2000.[10]

When using orthogonal collocation on finite elements it is also possible to show equivalence to the Galerkin method. For example, expand the solution as a polynomial within each element

$$\phi_l(s) = b_l + c_l s + s(1 - s) \sum_{i=1}^{N} a_{li} P_{i-1}(s) \tag{1.17}$$

We require continuity of the solution and first derivative at the ends of the element.

$$\phi_l(1) = \phi_{l+1}(0) \quad \text{or} \quad b_l + c_l = b_{l+1} \tag{1.18}$$

$$\Delta x_{l+1} \frac{d\phi_l}{ds}\bigg|_{s=1} = \Delta x_l \frac{d\phi_{l+1}}{ds}\bigg|_{s=0} \tag{1.19}$$

or

$$c_l - \sum_{i=1}^{N} a_{li} P_{i-1}(1) = c_{l+1} + \sum_{i=1}^{N} a_{l+1,i} P_{i-1}(0) \tag{1.20}$$

These equations effectively give b_l and c_l. The a_{li} are found by making the

residual, here just called $\mathscr{D}(s)$, orthogonal to the weighting function $\partial\phi_i/\partial a_{ii} = s(1-s)P_{i-1}(s)$ for each i.

$$\int_0^1 s(1-s)P_{i-1}(s)\mathscr{D}(s)\,ds = 0 \qquad i = 1, \ldots, N$$

Apply the quadrature formula, which is exact if $\mathscr{D}$ is a polynomial in s of degree N or less, to obtain

$$\sum_{j=1}^{N+2} W_j^{(N+2)} s_j(1-s_j)P_{i-1}(s_j)\mathscr{D}(s_j) = 0$$

This gives effectively $\mathscr{D}(s_j) = 0$ at $j = 2, \ldots, N+1$, and the conditions Equations 1.18 and 1.20 make the function and first derivative continuous at the element boundary. Thus the Galerkin method requires the collocation equations be satisfied. The reverse argument also holds. Thus, whenever the residual is of degree N in s and the trial function of degree $N+1$ in s is used, Equation 1.17, the Galerkin and orthogonal collocation methods on finite elements are identical.

There is one further feature of polynomial expansion on finite elements which should be examined: symmetry conditions. To illustrate the point, let us use the differential equation

$$\frac{d^2u}{dx^2} + \frac{a-1}{x}\frac{du}{dx} = f(u, x)$$

$$\left.\frac{du}{dx}\right|_{\substack{x=0 \\ u(1)=u}} = 0$$

where $a = 1, 2, 3$ for planar, cylindrical or spherical geometry. If we expand the solution in a power series, $u = \sum_{i=0}^{\infty} a_i x^i$, the boundary condition at $x = 0$ requires $a_1 = 0$. *If* we can prove that when $a_1 = 0$ then $a_3, a_5, \ldots,$ etc. are zero, too, then the solution can be expanded in even powers of x. This is done in Reference 1 and Reference 3, Section 5.1. The net effect of this simplification is that the number of terms needed in the expansion is reduced by a factor of 2. To achieve a trial function of order $2N$ in x we need only N polynomials in x^2 and N interior collocation points. If this simplification is not made, then we must use $2N-1$ interior collocation points. Now in the finite element expansions the differential equation will be transferred to

$$\frac{1}{\Delta x_l^2}\frac{d^2u}{ds^2} + \frac{a-1}{s\Delta x_l + x_l}\frac{du}{ds} = f(u, s\Delta x_l + x_l)$$

and the term $du/ds|_{s=0} = 0$ affects the solution in only the first element. The solution is not a symmetric polynomial in s, even though it is in x, since $x^2 = (s\Delta x_l + x_l)^2 = s^2\Delta x^2 + 2x_l\Delta x_l s + x_l^2$. Thus, by going to any finite element expansion for problems whose solution is symmetric we

automatically double the number of terms we must include to achieve the same level of approximation. The same results hold in problems whose solution includes only odd powers of x. As the number of dimensions increases the effect of symmetry is more pronounced. If symmetry exists in a three-dimensional problem, changing to a finite element approach (whether orthogonal collocation on finite elements or some other) will require 8 times as many points to achieve the same degree of polynomials. This is not to say we need 8 times as many points to achieve the same accuracy, since the possibility of placing small elements where needed may make possible improved accuracy with lower order polynomials. However, the symmetry of a problem is clearly an important consideration in choosing a method, and we illustrate this below for flow in a packed bed.

1.5 Orthogonal collocation (global and on finite elements) in two-dimensional problems

For two-dimensional problems the orthogonal collocation method is a straightforward extension of the method for one-dimensional problems. For a rectangular domain the trial function is the two-dimensional analogue of Equation 1.17.

$$u(x, y) = \left[b_1 + b_2 x + x(1 - x) \sum_{i=1}^{NX} a_i P_{i-1}(x) \right] \times \left[c_1 + c_2 y + y(1 - y) \sum_{i=1}^{NY} d_i P_{i-1}(y) \right]$$

The derivatives appearing in the differential equation are evaluated at the collocation points using Equation 1.9 in each direction.

For example, the equations for the fully-developed flow of a generalized non-Newtonian fluid in a rectangular duct are (considering only one quadrant of the duct)

$$0 = -\frac{\partial p}{\partial z} + \frac{\partial}{\partial x}\left(\eta(\mathrm{II})\frac{\partial w}{\partial x}\right) + \frac{\partial}{\partial y}\left(\eta(\mathrm{II})\frac{\partial w}{\partial y}\right)$$

or

$$0 = -\frac{\partial p}{\partial z} + \eta(\mathrm{II})\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right) + \frac{\partial w}{\partial x}\frac{\partial \eta}{\partial x} + \frac{\partial w}{\partial y}\frac{\partial \eta}{\partial y}$$

$$w = 0 \quad \text{on } x = a, \text{ all } y$$

$$w = 0 \quad \text{on } y = b, \text{ all } x$$

$$\frac{\partial w}{\partial x} = 0 \quad \text{at } x = 0, \text{ all } y$$

$$\frac{\partial w}{\partial y} = 0 \quad \text{at } y = 0, \text{ all } x$$

To examine the symmetry we see if the transformations $(w, x, y) \leftrightarrow (w, -x, -y)$ or $(w, x, y) \leftrightarrow (w, -x, y)$ change the differential equation. Since $2\text{II} = (\partial w/\partial x)^2 + (\partial w/\partial y)^2$ the equations are unchanged by these transformations, and the solution is thus a function of x^2 and y^2, not x and y. Thus we use symmetric polynomials

$$w(x, y) = \left[b + (1 - x^2)\sum_{i=1}^{NX} a_i P_i(x^2)\right]\left[c + (1 - y^2)\sum_{i=1}^{NY} d_i P_i(y^2)\right]$$

where the polynomials $P_i(x^2)$ are of order i in x^2 and are defined by

$$\int_0^1 (1 - x^2)P_i(x^2)P_j(x^2)\,dx = 0, \qquad i = 0, 1, \ldots, j - 1.$$

The trial function automatically satisfies the derivative condition along $x = 0$ and $y = 0$. The dimensions are also changed so that x and y both go from 0 to 1. The orthogonal collocation formulation of the problem is then

$$\begin{aligned} 0 = \frac{\partial p}{\partial z} &+ \eta(\text{II}_{ij})\left[\frac{1}{a^2}\sum_{k=1}^{NX+1} BX_{ik}w_{kj} + \frac{1}{b^2}\sum_{k=1}^{NY+1} BY_{jk}w_{ik}\right] \\ &+ \frac{1}{a^2}\left[\sum_{k=1}^{NX+1} AX_{ik}\eta(\text{II}_{kj})\right]\left[\sum_{k=1}^{NX+1} AX_{ik}w_{kj}\right] \\ &+ \frac{1}{b^2}\left[\sum_{k=1}^{NY+1} AY_{jk}\eta(\text{II}_{ik})\right]\left[\sum_{k=1}^{NY+1} AY_{jk}w_{ik}\right] \end{aligned}$$

with $w(x_i, y_j) = w_{ij}$, $i = 1, \ldots, NX$, $y = 1, \ldots, NY$ and

$$w_{i,NY+1} = w_{NX+1,j} = 0 \quad \text{all } i, j.$$

For non-linear, two-dimensional chemical reactor calculations we have used a Newton–Raphson method to solve non-linear algebraic equations similar to these,[11] but alternating direction methods are also possible.[12]

If the aspect (b/a) ratio is very large, the velocity profile will be very flat in the y direction. Then the global trial function would require a large number of terms, or NY, to approximate the solution. This is a situation when the method of orthogonal collocation on finite elements is useful. In the y direction, then, we use finite elements. To solve the algebraic equations, we use an alternating direction method: solve a succession of problems in the x direction, while keeping y fixed, and then solve a succession of problems involving the inversion of matrices as shown in Figure 1.1. To do this we need to linearize the equations for each iteration, which can be done by evaluating η at the previous iteration, or by using a Newton–Raphson method.

If the non-Newtonian fluid is such that flat velocity profiles are expected in both x and y direction, then orthogonal collocation on finite elements would be used in each direction. Again an alternating direction would be

used in order to permit the storage-saving features of the matrix shown in Figure 1.1. If the profile were not expected to be flat (say a Newtonian fluid with $b/a \sim 1$), then the global orthogonal collocation method would be used because of the $2^2 = 4$-fold reduction in number of collocation points when we include the symmetry of the problem.

1.6 Orthogonal collocation (global and finite elements) in time-dependent problems

Orthogonal collocation methods can be used for time-dependent problems, too, and reduce the problem to sets of ordinary differential equations in time. These equations can be solved using any one of several techniques for integration of ordinary differential equations as discussed in Reference 1, Chapter 5 and References 5, 13–15. Also, analogues of all the modifications of the Crank–Nicolson method for finite difference methods are applicable, while for two-dimensional problems alternating-direction methods are also possible.

Orthogonal collocation on finite elements also leads to ordinary differential equations in time. Explicit methods of integration lead to stability limitations related to Δx_i^2, as in finite difference methods. Implicit methods lead to matrices of the form of Figure 1.1 to invert at each time step (or perhaps only once if it is constant from one time to the next). Two-dimensional, time-dependent problems can be solved with alternating direction implicit methods.

1.7 Applications

A series of applications are considered to illustrate the comparison of global and finite element trial functions.

1.7.1 Entry-length problems

As a fluid moves into a duct, a boundary layer is formed near the walls and the thickness grows as the fluid moves down the duct. The solution to this problem exhibits large gradients, making useful finite element methods which can bunch the elements near the walls. We review first the global techniques and then consider finite element calculations.

In the momentum integral method, first presented by Schiller,[16] the boundary layer equations for a flat plate are integrated over the thickness of the boundary layer. A velocity profile is assumed and the boundary layer thickness can be calculated as a function of length down the duct by solving an ordinary differential equation. Campbell and Slattery[17] showed that more accurate results are achieved if the pressure drop is calculated from the kinetic energy balance including viscous dissipation. However, for some

non-Newtonian fluids, even this approach does not give accurate results (see Reference 1, p. 87). These methods are limited in usefulness because the accuracy is sometimes poor and cannot be estimated and a convergent process has not been defined to refine the calculation. In addition they are restricted to a few regular geometries, such as circular tubes or a duct between flat plates.

A convergent mathematical scheme for the flow problem can be applied as presented by Fleming and Sparrow.[18] They write the solution as the sum of the fully developed solution and an entry-region solution. The fully developed solution is found by using trial functions which satisfy the differential equation, which is easy to do since the differential equation for Newtonian fluids is Poisson's equation. Then the boundary conditions are applied by applying collocation on the boundary of the domain, which can be irregular. They use more collocation points than there are constants to fit in the trial function and so use a least squares collocation condition: minimize the sum of the collocation residuals on the boundary. The entry-region solution is then found from the solution to

$$\varepsilon(z)U\frac{\partial w^*}{\partial z} = \Lambda(z) + \nu\left[\frac{\partial^2 w^*}{\partial x^2} + \frac{\partial^2 w^*}{\partial y^2}\right]$$

where U is the mean velocity and the $\varepsilon(z)$ and $\Lambda(z)$ functions are found in the solution. Thus the solution includes inertial effects (with an approximation) and viscous terms in the axial direction, $\partial^2 w/\partial z^2$, are also neglected. The solution is expressed as an infinite series in h_i,

$$w^* = \sum c_i h_i e^{-\mu_i \xi}$$

$$\nabla^2 h_i + \mu_i h_i = 0, \qquad \frac{1}{\mu_i A}\oint \frac{\partial h_i}{\partial h}\,\mathrm{d}S = 1$$

Again the trial function satisfies the differential equation (with an as yet undetermined eigenvalue). The eigenvalue is found iteratively to satisfy the normalization condition and the boundary conditions are satisfied by a least squares collocation condition on the boundary. Since the entry-region solution is expressed as a series, the three-dimensional problem is reduced to a series of two-dimensional eigenvalue problems. Arbitrarily shaped ducts can be handled, although calculations are presented only for rectangular and triangular ducts. To achieve good accuracy near the inlet from 12 to 100 terms are required in the eigenfunction expansion, depending on the problem.

Atkinson and coworkers[19] solved the problem of slow flow of a Newtonian fluid using a finite element method. The problem was solved in terms of the stream function, so that second derivatives appeared in the functional, and quadratic shape functions were used on triangular elements. The number

of elements needed (as well as the number of eigenfunctions used by Fleming and Sparrow) depends on how close to the entrance one wants to resolve the velocity profile. For flow in a pipe the finite element calculation used 451 mesh points, in both radial and axial directions, but the closest profile to the inlet presented by Atkinson and coworkers is at length $z = 0{\cdot}1R$, where R is the pipe radius. By contrast, the expansion method of Fleming and Sparrow could be evaluated as close as $z = 0{\cdot}0006Re \,.\, D_h$ for rectangular ducts, using 100 eigenfunctions, where Re is the Reynolds number and D_h is the hydraulic diameter. For equilateral triangular ducts only 12 terms are needed. For an entry-length heat transfer problem for flow between parallel plates, Tay and Davis[20] used the finite element method with linear shape functions on triangles. They calculated to within $0{\cdot}0005Pe \,.\, h$, where Pe is the Peclet number and h is the thickness between plates; but the calculations still showed some error even for $21 \times 25 = 525$ mesh points.

Both global and finite element methods are applicable to arbitrary geometries perpendicular to the duct axis, but the eigenfunction techniques are probably more accurate for a given number of trial functions.

1.7.2 Boundary layer flows

In boundary layer flows the computations are complicated by the singularities of the solution and the semi-infinite domain. All the applications of the Method of Weighted Residuals known to the author have been with trial functions defined over the entire boundary layer rather than over finite elements, although the entry-length calculations cited above indicate finite element calculations might be possible.

One advantage of global expansion methods is that if the type of singularity is known it can sometimes be transformed away. As mentioned by Thompson,[21] and illustrated by him, if the solution varies wildly, an analytical transformation may be used to make the bad behaviour algebraically explicit; the new unknowns are then smooth. Some of the analyses of laminary boundary layers are attempts to do this.

In the method of integral relations (see, for example, Reference 1, p. 78) the boundary layer equations are integrated from the solid boundary to the edge of a subdomain. The subdomains usually are parallel to the shape of the body. The equations are then satisfied in subdomains, or strips running parallel to the body creating the boundary layer. In one sense the method is a finite element method in the transverse direction. The ordinary differential equations thus generated are integrated along the length of the body. As pointed out by Melnik and Ives[22] this method leads to equations which, if linearized, have both positive and negative eigenvalues. Furthermore, the magnitude of the eigenvalues increases rapidly as the number of strips increases. This makes the calculations difficult and the number of subdomains is usually limited to five or less. Melnik and Ives[22] indicate that an increase

in accuracy is possible if the location of the strips is not uniform, but the edges of the strip are placed at the roots to Chebyshev polynomials. They recommend for engineering calculations that two strips, so placed, are sufficient. For supersonic flows similar methods are applicable, but Holt and Ndefo[23] indicate they are too expensive. Chushkin,[24] on the other hand, maintains the scheme is efficient for supersonic flows about conical bodies, including three-dimensional cases.

Galerkin methods are also possible and have been developed by Dorodnitsyn[25,26] and Bethel.[27,28] The boundary conditions on velocity must be approached asymptotically so that the choice of trial functions may be difficult. To avoid this problem, a transformation is made

$$\theta(x, u) = (\partial u/\partial \eta)^{-1}$$

where the variables are θ—new dependent variable, x—lengthwise coordinate, u—lengthwise velocity, η—transverse coordinate. The full equations are summarized in Reference 1, p. 79. This method is efficient and often four term solutions are comparable in accuracy to 100 term finite difference solutions (Reference 1, p. 80). Unfortunately, it is not possible to ensure the completeness of the trial functions, owing to the transformation, and reversed flow formulations require different trial functions. Indeed for accelerating flows the trial function is $\theta(x, \mu) = \sum c_j(x)P_j(u)/(1 - u)$, where $P_j(u)$ is a polynomial in u. If the singularity in u is not handled correctly, the result may not converge to the solution. Thus, without considerable *a priori* knowledge about the solution, the accuracy cannot be guaranteed. This is both an advantage, if one is doing many calculations for a class of problems, and a disadvantage if one is doing many different kinds of problems.

The question of the proper singularity in Bethel's method is an important one. For free shear layers Stoy[29] applies the method and finds the nonlinear equations difficult to solve. The method was criticized by Wortman and Franks[30] as not being appropriate for an accurate solution and Stoy, in his reply, agreed. These conclusions apply to the type of trial function used and its singularity, rather than to the Method of Weighted Residuals as a whole.

To avoid this problem, MacDonald[31] applies a Crocco transformation in which the new independent variables become x and u while the new dependent variable is $\theta = (\partial u/\partial \eta)^2$. In this formulation there are no singularities and simple polynomial expansions in u can be used. The trial function is substituted in the differential equation, it is multiplied by a weighting function and the integrated result is set to zero. This process leads to nonlinear ordinary differential equations; if the problem admits a similarity solution, algebraic equations result.

Bossel[32] uses exponential trial functions, without making any transformation, and in compressible flow calculations[33] found that 5 terms in

the series compared in accuracy to 200 grid-point finite difference calculations. The calculations were faster per time step than finite difference calculations but required more steps due to the stiffness of the equations. Jaffe and Thomas[34] introduced yet another variation by applying quasi-linearization to the basic equations and solving the resulting linear equations using a series of Chebyshev polynomials. We note that the same equations result if the solution is expanded in the polynomials and then the Newton-Raphson method is applied. For the Falkner–Skan equation their method required about 10 times fewer terms than were needed in finite difference methods, but the computation times were comparable. In many ways this approach is comparable to applying orthogonal collocation and the corresponding generalization of applying orthogonal collocation on finite elements has not yet been applied.

Another interesting problem for which the Method of Weighted Residuals has been used to good advantage is the treatment of laminar flow in strongly curved tubes.[35] At high Reynolds number, boundary layers are formed, and these are treated using the integral methods described in the previous section. For lower Reynolds number the velocities are expanded in a Fourier series in the angular variable. The trial function is substituted into the equations and the coefficients of $\sin n\phi$ and $\cos n\phi$ are set to zero. This is a Fourier series method, but can also be viewed as a collocation method with Fourier series expansion functions. The ordinary differential equations in r are then solved. In this way the rather formidable two-dimensional, three-velocity-component, flow problem is reduced to manageable proportions.

It is clear from this summary that applications to boundary layer flows using global trial functions have been successful in varying degrees. Finite element methods are feasible, as illustrated by other papers in this book. Certainly the orthogonal collocation method on finite elements is one candidate for calculation, with larger elements far from the body to handle the infinite domain and perhaps generating differential equations in the lengthwise direction. Whether finite element methods are competitive in terms of efficiency of computation (accuracy, computation time and storage) remains an open question.

1.7.3 Flow in packed beds

One of the strengths of the finite element method is its adaptability to different and complicated geometries. This feature is especially useful when one wants to solve similar problems, differing only in geometry, such as in design studies. If the problem has a great deal of symmetry, however, global methods are able to reduce the number of trial functions needed by taking that symmetry into account. Finite element methods, however, can take the symmetry into account (by setting derivatives to zero, for example) only in the elements nearest the line of symmetry. An example of the efficiency

of global methods is presented for the slow flow of a Newtonian fluid through a bed of solid spheres packed in a simple cubic array.

Sørensen[36] solved the three-dimensional flow problem given by

$$\mu \nabla^2 \mathbf{v} = -\nabla p$$

with $\mathbf{v} = 0$ on the boundary of the spheres. The equations and geometry, and hence the solution, exhibit the symmetry shown in Table 1.3. The average flow is in the z direction, which is parallel to one orientation of the spheres.

The three-dimensional velocity is expressed as

$$\mathbf{v} = \nabla F \times \nabla G$$

which automatically satisfies the continuity equation.

Table 1.3 Symmetry conditions for flow in simple cubic packed bed*

Transformation		Functions which are unaffected	Functions which change sign
(1)	$x \to -x$	v_y, v_z, p	v_x
(2)	$y \to -y$	v_x, v_z, p	v_y
(3)	$z \to -z$	$v_z, p \to 2p_0 - p(x, y, -z)$	v_x, v_y
	Other transformations		
(4)	$(x, y) \to (y, x)$	$v_x \to v_y$ v_z, p unchanged	
	Periodicity conditions		
(5–7)	$\mathbf{v}(x, y, z) = \mathbf{v}(x + 2i, y + 2j, z + 2k)$ $p(x, y, z) = p(x + 2i, y + 2j, z + 2k) - 2k\,\Delta p$ i, j, k = any integer values		

* The spatial dimensions have been non-dimensionalized in terms of the sphere radius.

The symmetry is included in the trial functions by a change of coordinates. The coordinate ξ_2 is given by

$$\xi_2 = 2 \frac{\sum_{\pm j = 1, 2, \ldots} j(1 - 1/P_j)}{\sum_{\pm j = 0, 1, \ldots} (1 - 1/P_j)}$$

$$P_j = \prod_i \prod_{\pm k = 0, 1, \ldots} [1 - \exp(-w1 d_{ijk})][1 - \exp(-w2 d_{ijk})]$$

$$\pm i = 1, 3, 5, \ldots, j \text{ odd}$$

$$\pm i = 0, 2, 4, \ldots, j \text{ even}$$

$$(d_{ijk} + 1)^2 = (x - 2i)^2 + (y - 2j)^2 + (z - 2k)^2$$

Three other coordinate lines are obtained from the same expressions using various interchanges of indices. The pair (ξ_1, ξ_2) give coordinate lines

which are nearly perpendicular and cover the region (in the x–y plane) between the four spheres. The other pair (ξ_3, ξ_4) curve in the opposite sense and both grids are needed to obtain the full symmetry.

The trial functions are written as Fourier series

$$F_1 = \xi_1/2 \qquad G_2 = \xi_2/2$$

$$G_1 = \xi_2/2 + 2\sum C_m \cos(j\pi\xi_1) \sin(i\pi\xi_2) \cos(k\pi z)$$

$$F_2 = \xi_1/2 + 2\sum C_m \sin(i\pi\xi_1) \cos(j\pi\xi_2) \cos(k\pi z)$$

$$\mathbf{v}_{12} = \nabla F_1 \times \nabla G_1 + \nabla F_2 \times \nabla G_2$$

and this construction for F and G keeps the problem linear in the unknowns, $\{C_m\}$. A similar expression is written to obtain $\mathbf{v}_{34}$ and to obtain the full symmetry we use

$$\mathbf{v} = \mathbf{v}_{12} + \mathbf{v}_{34}$$

The collocation points are spaced somewhat uniformly between the spheres in each x–y plane. The residuals are set to zero and the equations solved. The pressure drop was calculated by evaluating the viscous dissipation, with very good accuracy. For a total number of unknowns of 30, 42 and 54 the pressure drop differed by only $\pm 0{\cdot}04\%$. Using that answer as the exact result, the calculations for $n = 2$ had an error of $0{\cdot}7\%$ while $n = 8$ gave $0{\cdot}4\%$ error. The fact that 1% accuracy can be achieved with only 2 terms is a result of including the eight-fold symmetry in the trial functions. If a finite element or finite difference calculation were used we would need about 2^8 times as many mesh points or grid points. This is a dramatic illustration of the power of global trial functions in special cases.

1.7.4 Newtonian fluids flowing past spheres and cylinders

Flow past spheres and cylinders at finite Reynolds numbers is a problem which has been solved many times using different methods. The Galerkin method has been applied to flow past a sphere using a trial function which contains the Stokes solution as a special case[37]

$$\psi(r, \theta) = P_1(r) \sin^2\theta + P_2(r) \sin^2\theta \cos\theta$$

With only two terms in the θ direction, good accuracy could not be expected. At $Re = 100$ the solution was compared to a finite difference solution (using 60 annular grid points and 78 radial points). The Galerkin method using the crude velocity profile gave reasonable accuracy of average quantities, such as drag coefficient, but pointwise values of separation angle, pressure profile on the sphere, etc., were not well determined.

Other authors have expanded the solution in Fourier series (see Reference 38, for cylinders) and Legendre polynomials in $\cos\theta$ (see References 39 and 40 for spheres and 41 for cylinders). The trial function is substituted into the

differential equation and the coefficient of each angular function in the trial function is set to zero. This can be interpreted as a collocation method in the θ direction. All these authors then used various finite difference methods to solve the set of ordinary differential equations in the r direction. The calculations could not be taken to high Reynolds number because the number of modes needed increased dramatically with Reynolds number. For the sphere,[39] 16 modes were necessary for very accurate solutions at $Re = 40$. For the cylinder[41] 80 modes were used with $Re = 100$. Collins and Dennis[41] also solved the problem of an impulsively started cylinder and, for small times, transformed the problem using boundary layer coordinates to obtain accurate solutions.

The author and one of his students (Ronald Andermann) have applied orthogonal collocation on finite elements to flow past a sphere. The problem was formulated in terms of the stream function and vorticity.

$$\sin\theta\left[\frac{\partial\psi}{\partial r}\frac{\partial}{\partial\theta}\left(\frac{\zeta}{r^2\sin^2\theta}\right)-\frac{\partial\psi}{\partial\theta}\frac{\partial}{\partial r}\left(\frac{\zeta}{r^2\sin^2\theta}\right)\right]=\frac{2}{Re}E^2\zeta$$

$$r\sin\theta\zeta = E^2\psi$$

$$E^2=\frac{\partial^2}{\partial r^2}+\frac{\sin\theta}{r^2}\frac{\partial}{\partial\theta}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\right)$$

In the θ direction each variable was expanded in sine functions, while the r direction was divided up into elements and orthogonal collocation was applied in each element. The equations were solved iteratively using an alternating direction method. For a given stream function, the vorticity was found from the first equation by successive sweeps in the θ and then the r direction. When sweeping in the θ direction (constant r) the inertial terms involving $\partial\zeta/\partial\theta$ were put on the side with $\partial^2\zeta/\partial\theta^2$ and when sweeping in the r direction the $\partial\zeta/\partial r$ and $\partial^2\zeta/\partial r^2$ terms were used as unknowns in the iteration. When this problem had converged, the next equation was solved for stream function, for the given vorticity. This was also done using an alternating direction method. In this way the storage requirements for the matrices to invert were no larger than needed to solve ordinary differential equations using orthogonal collocation on finite elements. The calculations are not yet complete, but the results to date indicate the method gives very accurate answers; the practical upper limit in Reynolds number, however, has not yet been determined.

The finite element method has been applied to the flow past a cylinder for Reynolds numbers up to 100 by Taylor and Hood.[42] Their recommended procedure leaves the equations in terms of the primary variables, velocity and pressure, and keeps the time derivatives in order to integrate to steady

state. The Galerkin method was used on elements with trapezoidal bases and apparently quadratic shape functions.* Taylor and Hood found that the non-linear inertial terms had to be included in the linear iteration scheme, rather than simply be evaluated at the old iteration, in order to have stable calculations. Unfortunately, for the cylinder problem the detailed features like drag coefficient and separation angle were not reported, so that comparisons cannot be made concerning accuracy. The computation time was large, being greater than 100 minutes for $Re = 100$ on an ICL 1905E computer. The work does, however, show the efficacy of the finite element method for Reynolds numbers this high. This paves the way for other applications, like flow past banks of cylinders, where the ease of handling irregular geometries will be especially useful.

1.7.5 Reservoir engineering problems

In the section on trial functions, considerable discussion was given to convergence results for various types of polynomials for one-dimensional problems. The same polynomials can be used in two dimensions, making the methods finite elements on square bases. Applications like this have been made in the field of reservoir engineering problems and the results have been compared to finite difference results, which is the usual method of calculation. The comparisons give some interesting results.

Price and Varga[43] solved a linear time-dependent problem in one dimension, for parameters giving rise to a moving wave front in the solution. They used the Galerkin method with piecewise linear, cubic and quintic trial functions, as well as one calculation with piecewise linear functions everywhere except near the wave front where quintic polynomials were used. The results showed that the computation time was much less than that for finite difference calculations, sometimes 10 times less, and that the improvement was best when solutions were desired of high accuracy.

The next comparison is for a non-linear problem, but still for one space dimension and time. Culham and Varga[44] used smooth linear and cubic Hermite polynomials, non-smooth cubic polynomials and cubic spline polynomials. These trial functions were used along with the Galerkin method. Cubic spline functions were also used with a collocation method. The results were compared based on the pointwise error, but a bias was introduced into the results. The finite difference results were compared based on the error at the grid points, whereas the Galerkin results and collocation results were based on the error throughout the entire domain. The convergence results cited above indicate that the solution in the orthogonal collocation method is more accurate at the collocation points than

* The shape functions are defined for another problem in the same paper, but not for flow past a cylinder.

globally (see, particularly, Reference 9), so that the comparison of the spline collocation method may be comparing the least accurate part of the collocation solution with the most accurate part of the finite difference solution. The Galerkin results may not be discriminated against, since the rate of convergence applies globally. The authors also compared four different methods of handling the time-dependent calculations. They found that the Galerkin results were always inferior to the finite difference results when comparing computation time to achieve a specified accuracy. The cubic spline collocation results were more competitive, but were faster than the finite difference results only for the most accurate solutions determined. The reason given for the dramatic difference in conclusion reached in this non-linear problem, compared to the linear problem, was that a large fraction of the computation time was to evaluate quadratures to be used in the Galerkin method. Since the problem was non-linear, these quadratures had to be recomputed at each time step and the entire method became inefficient. We note also that cubic splines give convergence as Δx^2 whereas cubic polynomials in orthogonal collocation gives convergence as Δx^4.

Two-dimensional calculations are reported by McMichael and Thomas[45] for the full scale, three phase production of an oil field (non-linear equations, parabolic in time, elliptic in two space dimensions). They used both linear and cubic polynomials in each direction on finite elements with square bases. They concluded that the Galerkin method was feasible to apply and in many cases gave results which were superior to those from finite difference schemes and gave more realistic profiles. For a given time step the Galerkin method requires significantly more machine time, but larger time steps are allowed; the net effect was that the finite difference results took from $\frac{1}{2}$ to $\frac{6}{5}$ times as much computer time as the Galerkin method. The Galerkin method also gave less numerical dispersion than the finite difference methods.

These results suggest that for certain non-linear problems the finite element method may not be competitive with finite difference methods in terms of computation time, because of excessive time spent calculating integrals in the Galerkin method. This same problem does not arise in the method of orthogonal collocation on finite elements because the collocation method is used, but the rate of convergence is the same as the Galerkin method when Gaussian quadrature points are used. Consequently this is a type of problem for which the marriage of orthogonal collocation and finite elements may provide a solution to an important difficulty.

1.7.6 Non-Newtonian fluids

When the fluid is no longer Newtonian, the viscosity is a function of the velocity gradient and the integrals in a variational principle (if one exists) or the Galerkin method become difficult to evaluate (e.g. Equation 1.4). Some recent finite element work has tackled these problems using a viscosity

which was constant within an element, but which varied from element to element.[46–48] In these cases linear shape functions were used for velocity and pressure (or quadratic functions for stream function) so that the velocity gradients were constant within triangular elements. Then the viscosity function is actually constant within an element. The calculations of Taylor and Hood,[42] however, used quadratic trial functions for Newtonian fluids. If these shape functions were used for non-Newtonian problems, the viscosity would vary over the element, the stiffness matrices would have to be re-calculated at every iteration and a finite element solution might run into the same problem found in the reservoir engineering calculations: the finite element may not be competitive with finite difference methods in terms of computation time for a given accuracy.

Another feature of interest is more general constitutive equations. The power law fluid is a common one and has

$$\boldsymbol{\tau} = -2K(2d_{ij}d_{ji})^{n-1/2}\mathbf{d}$$

Polymer flows are usually viscoelastic, however, leading to constitutive equations of the form, e.g.

$$(1 + \lambda_1 F)\boldsymbol{\tau} = 2\mu_0(1 + \lambda_2 F)\mathbf{d}$$

$$F\boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u}\,.\,\nabla\boldsymbol{\tau} + \mathbf{w}\,.\,\boldsymbol{\tau} - \boldsymbol{\tau}\,.\,\mathbf{w} - (1 + \varepsilon)(\mathbf{d}\,.\,\boldsymbol{\tau} + \boldsymbol{\tau}\,.\,\mathbf{d}) + \tfrac{2}{3}(1 + \varepsilon)(\mathbf{d}\,.\,\boldsymbol{\tau})\mathbf{1}$$

The applicability of finite element methods (or any other method) has yet to be shown, but the possibility of using both stress and velocity shape functions in the finite element method may be useful.

Global trial functions have been applied to non-Newtonian fluids, particularly for flow around spheres and flow through ducts (see Reference 1 for references), but rarely are the solutions done numerically and continued until numerical convergence was obtained. The method of orthogonal collocation on finite elements might be a good compromise for these problems: by avoiding the calculation of integrals but retaining some of the convenient features of finite element methods.

1.7.7 Flow with free boundaries

When a free boundary exists, on which the normal and viscous stresses must be balanced between the two fluids, the calculation is complicated by the unknown position of the boundary. The finite element method is ideally suited to such problems: by assuming the shape of the boundary, solving the problem and then correcting the shape and repeating the calculation, the location of the boundary can be determined. The advantage of the finite element method in handling diverse geometries is especially useful here. Thompson and coworkers[46] treated a power law fluid squeezed between two

flat plates, with the fluid exposed to air in between the plates. Chan and Larock[49] applied the finite element method to an inviscid, irrotational fluid out of an orifice. The viscous problem is much more complicated, of course, but the iterative method of finding the shape of the jet was verified. The author is currently applying the method of orthogonal collocation on finite elements to problems involving both non-Newtonian fluids and free boundaries.

1.8 Conclusion

The classical Method of Weighted Residuals, in which the trial functions are defined over the entire domain, and the finite element method, which uses variational or Galerkin principles but utilizes trial functions defined over finite elements, are similar in many respects. The finite element method is preferred when there are rapid changes of the solution, or complicated geometries. In other situations the Method of Weighted Residuals, with global trial functions, is preferred for its very rapid convergence and savings in both storage and computation time. In addition the analytic form of the solution is convenient in many situations. The method of orthogonal collocation on finite elements is a combination of both methods. By using a collocation principle, the quadrature evaluation is eliminated, giving rise to time savings in non-linear problems. By using orthogonal collocation, the method converges as fast as a Galerkin method (in certain cases). So far the method has only been applied to problems with some symmetry, so that diverse geometries have not yet been handled. Orthogonal collocation on finite elements provides a bridge between methods using global and finite element trial functions and the limits of the method are yet to be defined. A broad outlook of weighted residual methods and finite element methods leads to interesting and useful comparisons and interrelations which reveal the advantages of each approach.

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