

REVIEW: FORMULATING EFFICIENT FINITE-ELEMENT CODES FOR FLOWS IN REGULAR DOMAINS

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SUMMARY

Many fluid flow problems of current interest occur in domains that are mappable to a rectangle or a box; conformal mappings are particularly useful in this regard. We are concerned here with the efficient solution of such problems using finite elements. The central issue is the element choice, and this issue is addressed in terms of operation counts, computer memory and I/O requirements, and the extent to which code vectorization is possible. It is concluded that rectangular (box) elements generally lead to more efficient algorithms than triangular (tetrahedral) elements. A synthesis of algorithms, based on bilinear (trilinear) elements, is presented. The algorithms have the attributes of simplicity, accuracy, stability and straightforward incorporation of boundary conditions. For bilinear and trilinear elements, it is found that product and first-derivative terms are well-handled by the Galerkin FE method, but that it is advantageous to go outside of the Galerkin framework when treating second-derivative terms. It is particularly important to consider the form of the governing equations, *vis-à-vis* the choice of staggered, non-staggered and/or mixed-order elements, and to choose an appropriate time scheme. The described techniques have been successfully applied to a variety of problems in regular domains, including the solution of the three-dimensional time-dependent hydrostatic primitive equations; these are stiff and include first and second derivative terms, non-linearities and variable coefficients due to a conformal mapping.

KEYWORDS Separable Basis Tensor Product Vectorized code Finite Element

1. INTRODUCTION

Many fluid flow problems of current interest occur in regular domains. In the context of this paper we define a regular domain to be one that can be mapped (conformally or otherwise) to either a rectangle or a box. This class of problem is quite large and includes flow in a periodic channel, flow around obstacles in an unbounded domain, flow within a rotating annulus and simulation of the earth's atmosphere including orographic effects. Often, when one is interested in understanding more about physical phenomena (e.g. convection studies), the choice of geometry is quite arbitrary and is frequently taken to be regular for both convenience and efficiency. It is clear that there are many problems which are not included in this class (e.g. flow of the world's oceans), but we restrict ourselves here to flows in regular domains since they nevertheless constitute a widely used class of problems.

The central issue when formulating a finite-element (FE) flow model is the choice of elements, since this choice has a very direct impact on the accuracy, stability, computational efficiency and simplicity of a given formulation. We address this issue in terms of (i) operation counts, (ii) the amount of memory and I/O required and (iii) the degree of code vectorization that is possible. Illustrative examples are mostly drawn from the atmospheric sciences because of the author's

interests, but the major part of the material presented here is a synthesis of efficient algorithms for flow problems in regular domains.

To help clarify the use of the presented algorithms, we relate them to a non-trivial concrete example drawn from meteorology and oceanography, the shallow-water equations on a rotating sphere. These equations, although simple in form, are nevertheless very useful for illustrative purposes since they include time-dependence, two space dimensions, first and second derivatives, non-linear terms, stiffness and variable coefficients due to a co-ordinate transformation (mapping). On a polar-stereographic projection, true at 60° N, they are¹

$$\zeta_t/S = -[(QU)_x + (QV)_y], \quad (1)$$

$$D_t/S + \phi_{xx} + \phi_{yy} = (QV - K_x)_x - (QU + K_y)_y, \quad (2)$$

$$\phi_t/S + \Phi_0 D/S = -[(\phi U)_x + (\phi V)_y], \quad (3)$$

where

$$\zeta = S(V_x - U_y) = \text{relative vorticity}, \quad (4)$$

$$D = S(U_x + V_y) = \text{divergence}, \quad (5)$$

$$Q = \zeta + f = \text{absolute vorticity}, \quad (6)$$

$$K = S(U^2 + V^2)/2 = \text{kinetic energy}, \quad (7)$$

$$U = u/m, V = v/m \quad \text{and} \quad S = m^2.$$

Here, x and y are the co-ordinates of the projection, u and v are the components of the wind vector along the axes of the co-ordinate system, ϕ is the perturbation geopotential height of the free surface about its mean value (Φ_0), $m = (1 + \sin 60^\circ)/(1 + \sin(\text{latitude}))$ is the map-scale factor, f is the Coriolis parameter and U and V are termed the wind images. Decomposing the wind images in terms of a velocity potential χ and a stream function ψ , we have

$$U = \chi_x - \psi_y, \quad (8)$$

$$V = \chi_y + \psi_x, \quad (9)$$

which lead to the relations

$$\psi_{xx} + \psi_{yy} = \zeta/S, \quad (10)$$

$$\chi_{xx} + \chi_{yy} = D/S, \quad (11)$$

For a contained flow, $\psi = 0$ and $\nabla\chi \cdot \boldsymbol{\eta} = 0$ on the boundary, where $\boldsymbol{\eta}$ is the normal vector at boundary.

Equations (1) and (2) are derived from the momentum equations and (3) is the continuity equation. For the corresponding problem in a plane geometry, the equations remain unchanged, except that $m = s = 1$ and f is constant.

In section 2 we examine the impact that the element choice has on the structure of the matrices which result from application of the Galerkin finite-element method (GFEM), by comparing the computational effort required to evaluate derivatives and products when using (linear) rectangular and triangular elements. The key issue here is the efficient solution of the ‘mass-matrix problem’.

A breakdown of the remainder of the paper is: section 3—element order, spatial evolutionary error and code modularity; section 4—staggered, non-staggered and mixed-order elements, and the form of the governing equations; section 5—stability; section 6—miscellaneous considerations; section 7—time schemes and section 8—principal conclusions.

2. COMPUTING DERIVATIVES AND PRODUCTS—THE ‘MASS-MATRIX PROBLEM’

The essence of the GFEM^{2,3} is to

- (i) expand the dependent variables of the problem in terms of a set of basis functions, each of which is a low-order polynomial of compact support (i.e. non-zero only over a small subdomain called an element)
- (ii) insert these expansions into the governing equations and orthogonalize the error to the basis.

The first task is to geometrically subdivide the domain of the problem into a set of overlapping subdomains, and to examine the impact on efficiency of the choice of subdivision. To illustrate this point, let us examine the simple (but fundamental) operations of calculating first derivative and product terms over a rectangular domain, and contrast the impact of a subdivision of the domain into rectangles (Figure 1(a)) with that of arbitrarily chosen triangles (Figure 1(b)) when using linear elements. Clearly triangularization is more general than rectangularization, being applicable to an arbitrary polyhedral domain, but here we only concern ourselves with problems in a Cartesian geometry. The key issues for problems that are mappable to a Cartesian geometry are

- (i) can we afford the generality of triangles in comparison to rectangles?
- (ii) does either offer any advantage over competing methods such as finite differences?

As we will see, the answer to (i) is an overwhelming no, whereas the answer to (ii) is a qualified yes for rectangular FEs.

It remains to define the basis functions. For both triangular and rectangular elements we associate a basis function with each and every vertex (or node). The basis function associated with a given node is defined to be unity at the node, to vary linearly to zero at neighbouring nodes and to be identically zero elsewhere. In Figure 1, the given node is denoted by a square (■) and neighbouring nodes by circles (●); the associated basis function is unity at squares (■), zero at circles (●) and non-zero only within the hatched areas. For a rectangular element (Figure 1(a)), the algebraic variation of the basis function over a hatched

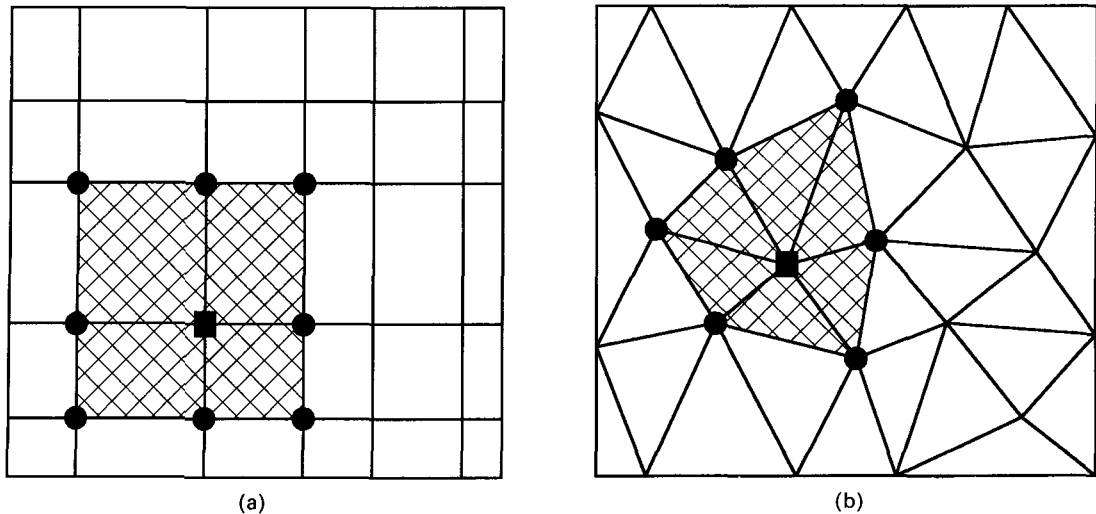


Figure 1. Two subdivisions of a rectangular domain: (a) rectangles, and (b) triangles. Basis functions associated with square nodes (■) are unity at these nodes (■), vary linearly to zero at neighbouring circular nodes (●), and are zero outside hatched areas

rectangle is $(a + bx)(c + dy)$ where a, b, c and d are determined such that the basis function is unity at the given node and zero at the other three nodes of the rectangle. Similarly for triangular elements (Figure 1(b)), except that the algebraic variation within a hatched triangle is $a + bx + cy$, since a triangle has one less node than a rectangle. For both rectangular and triangular elements the basis is an interpolatory one, since the coefficients in the expansion of a function in terms of the basis are just the values of the function at the nodes.

First derivatives

Consider the problem of evaluating

$$v = u_x, \quad (12)$$

where u is known at the set of nodal points and we require values of v at these nodal points. The first step in the FE treatment of this problem is to expand u as

$$u(x, y) = \sum_i u_i e^i(x, y), \quad (13)$$

where $e^i(x, y)$ is the basis function associated with the i th node (assuming some ordering of nodes), the sum over i is the sum over all nodes and u_i is the value of $u(x, y)$ at the i th node: v is also expanded in a similar manner. After insertion of these expansions into (12) and orthogonalization of the error to the basis (by multiplying by an arbitrary basis function and integrating over the domain), we obtain a set of linear equations of the form

$$\mathbf{P}\mathbf{v} = \mathbf{Q}\mathbf{u}, \quad (14)$$

where \mathbf{u} and \mathbf{v} are vectors of nodal values, \mathbf{P} and \mathbf{Q} are large sparse matrices and \mathbf{P} is often referred to as the mass matrix or projection matrix. For rectangular elements with the usual row-wise ordering of elements, both \mathbf{P} and \mathbf{Q} are block tridiagonal and each block is itself tridiagonal. For triangular elements there is no natural ordering and the structure will depend on the particular ordering chosen.

For *rectangular* elements, (14) may be written explicitly at the point (x_m, y_n) of the mesh (Figure 1(a)) as

$$\begin{aligned} & (1/36)[h_{m-1}k_n v_{m-1, n+1} + 2(h_{m-1} + h_m)k_n v_{m, n+1} \\ & \quad + 2h_{m-1}(k_{n-1} + k_n)v_{m-1, n} + 4(h_{m-1} + h_m)(k_{n-1} + k_n)v_{m, n} + 2h_m(k_{n-1} + k_n)v_{m+1, n} \\ & \quad + h_{m-1}k_{n-1}v_{m-1, n-1} + 2(h_{m-1} + h_m)k_{n-1}v_{m, n-1} + h_mk_{n-1}v_{m+1, n-1}] \\ & = (1/12)[k_n(u_{m+1, n+1} - u_{m-1, n+1}) + 2(k_{n-1} + k_n)(u_{m+1, n} - u_{m-1, n}) \\ & \quad + k_{n-1}(u_{m+1, n-1} - u_{m-1, n-1})], \end{aligned} \quad (15)$$

where $h_m = x_{m+1} - x_m$ and $k_n = y_{n+1} - y_n$. The evaluation of the right-hand side of (15) is explicit and straightforward to calculate, but it is not immediately clear how to solve efficiently for $v_{m, n}$ given the implicit way in which it appears.

The brute-force method of multiplying the right-hand side of (15) by the inverse of \mathbf{P} is clearly not viable since this requires $O(M^2 N^2)$ arithmetic operations and $O(M^2 N^2)$ words of storage for an $M \times N$ mesh, even when \mathbf{P}^{-1} has been precalculated. The operation count and memory requirements may both be reduced to $O(M^2 N)$ if a ‘banded-solver’ is used that exploits the fact that the elements of \mathbf{P} are zero everywhere outside the tridiagonal band of blocks centred on the diagonal. Although this is better, it is still a factor of $O(M)$ more expensive than the theoretical

optimum of $O(MN)$ operations and storage. Since $M \sim 50\text{--}100$ in many applications, this is still a very expensive proposition, both in terms of arithmetic operations and storage. Cullen⁴ proposed a method that uses a truncated series to obtain an approximate solution, the accuracy of the solution depending on the number of terms taken. This method has the advantages of reducing memory requirements to optimum order and decreasing the operation count, but has the disadvantages of not being exact, not having an optimal operation count and only working for uniform grids. Iterative methods suffer from similar deficiencies except that they are applicable to non-uniform Cartesian meshes.

It must be emphasized that it is extremely important to be able efficiently to solve (14) if the FE method is to be competitive with the finite-difference (FD) method, since \mathbf{P} is the identity matrix for FD methods and the problem is then trivial. The matrix \mathbf{P} in the finite-element literature is often replaced by the identity matrix (or mass-lumped in FE parlance), but as we shall see later, this may be undesirable since it can lead to a significant reduction in the accuracy of the method.

Efficient solution of the 'mass-matrix problem' for rectangular elements

An efficient solution algorithm for (14) is easily derived for the rectangular element case (but *not* the triangular element case). This algorithm, even though it first appeared in the meteorological literature in 1977,¹ was not widely used until relatively recently. In the engineering literature it has been used in conjunction with approximate factorization techniques⁵⁻⁸ and is often referred to as the tensor product method. The essence of the solution algorithm is to

- (i) Solve the set of one-dimensional tridiagonal problems

$$\mathbf{P}^x \mathbf{s}_n = \mathbf{r}_n, n = 1, 2, \dots, N, \tag{16}$$

for \mathbf{s}_n along lines of constant y (i.e. n fixed) using Gaussian elimination,⁹ where

$$\mathbf{r}_n = \begin{bmatrix} r_{1,n} \\ r_{2,n} \\ \vdots \\ r_{M-1,n} \\ r_{M,n} \end{bmatrix}, \mathbf{s}_n = \begin{bmatrix} s_{1,n} \\ s_{2,n} \\ \vdots \\ s_{M-1,n} \\ s_{M,n} \end{bmatrix}, \mathbf{P}^x = \frac{1}{6} \begin{bmatrix} 2h_1 & & & & & \\ & h_1 & & & & \\ h_1 & 2(h_1 + h_2) & & & & \\ & & h_2 & & & \\ & & & \ddots & & \\ & & & & h_{M-2} & \\ & & & & & 2(h_{M-2} + h_{M-1}) & & \\ & & & & & & h_{M-1} & \\ & & & & & & & h_{M-1} \\ & & & & & & & 2h_{M-1} \end{bmatrix}$$

and $r_{m,n}$ is the right-hand side of (15).

- (ii) Solve the set of one-dimensional tridiagonal problems

$$\mathbf{P}^y \mathbf{v}_m = \mathbf{s}_m, m = 1, 2, \dots, M, \tag{17}$$

for \mathbf{v}_m along lines of constant x (i.e. m fixed), again using Gaussian elimination, where

$$\mathbf{v}_m = \begin{bmatrix} v_{m,1} \\ v_{m,2} \\ \vdots \\ v_{m,N-1} \\ v_{m,N} \end{bmatrix}, \mathbf{s}_m = \begin{bmatrix} s_{m,1} \\ s_{m,2} \\ \vdots \\ s_{m,N-1} \\ s_{m,N} \end{bmatrix}, \mathbf{P}^y = \frac{1}{6} \begin{bmatrix} 2k_1 & & & & & \\ & k_1 & & & & \\ k_1 & 2(k_1 + k_2) & & & & \\ & & k_2 & & & \\ & & & \ddots & & \\ & & & & k_{N-2} & \\ & & & & & 2(k_{N-2} + k_{N-1}) & & \\ & & & & & & k_{N-1} & \\ & & & & & & & k_{N-1} \\ & & & & & & & 2k_{N-1} \end{bmatrix},$$

The above algorithm requires $O(MN)$ operations and $O(MN)$ storage (i.e. it is of optimum order), is stable to round-off error, gives the *exact* solution (to within round-off error) to the set of linear equations defined by (15), easily generalizes to three dimensions, and includes the equations appropriate to boundary points.

To put this in the context of an application code, let $M = N = 100$, and then the number of arithmetic operations and words of storage is $O(10^4)$ which poses no problem for a large mainframe computer. On the other hand, a ‘banded solver’ would require $O(10^6)$ arithmetic operations and words of storage, which is two orders of magnitude more voracious. Of these two drawbacks (namely the larger number of arithmetic operations and the larger storage requirements) perhaps the most severe is the storage requirement, since the problem is unlikely to fit in (computer) memory. This then results in the need to perform extensive I/O to and from mass storage¹⁰ and the code becomes I/O bound (i.e. the CPU will spend most of its time waiting for operands to arrive from mass storage).

Regarding vectorization (a very important aspect of coding for supercomputers) the algorithm appears, at first sight, not to vectorize, because Gaussian elimination is a set of recursive operations. However, by performing each operation of Gaussian elimination in parallel for all members of the set of tridiagonal problems in x or y (as the case may be), a vectorizable operation is established in the transverse direction, and the algorithm is thus fully vectorizable.

It is interesting to note that even though the above algorithm is of optimal order, it can nevertheless still be improved upon in the context of taking a derivative (e.g. when computing U and V from χ and ψ using (8) and (9), by exploiting the particular form of the right-hand side of (15). It can be shown that (15) may be rewritten as

$$(1/6)[h_{m-1}v_{m-1,n} + 2(h_{m-1} + h_m)v_{m,n} + h_mv_{m+1,n}] = (1/2)(u_{m+1,n} - u_{m-1,n}). \quad (18)$$

The algorithm thus reduces to solving (18) for $v_{m,n}$ along lines of constant y (i.e. constant n). This is equivalent to solving a set of one-dimensional FE problems, holding y fixed, and is consistent with the underlying mathematics where the x -derivative at a point is obtained by a limiting process holding y fixed. This consistency does not obtain with triangular elements.

For *triangular* elements the best we can usually do for the solution of the mass-matrix problem is to either use a ‘banded-solver’ or an iterative method, both of which are considerably (typically at least an order of magnitude) more expensive than the algorithm for rectangular elements defined by (16) and (17).

Comparison with FD evaluation of first derivatives

Let us compare the efficiency and accuracy of evaluating a derivative using linear rectangular elements with those using second and fourth-order finite differences. First, we note that on any *uniform* subdomain (i.e. $h_{m-1} = k_{n-1} = h = \text{constant}$), equation (18) gives an $O(h^4)$ accurate estimate for the derivative at the nodes, a result often referred to in the literature as super-convergence at nodes.² Triangular elements generally give $O(h^2)$ accuracy and furthermore the solution of (14) is far more costly, so that we pay considerably more to get considerably less. The second-order centred finite-difference solution amounts to replacing the left-hand side of (18) by $hv_{m,n}$ (mass-lumping), and in comparison with rectangular FEs we find there is less computational effort (approximately a factor 2.5) but considerably less accuracy [$O(h^2)$ compared to $O(h^4)$]. On the other hand, fourth-order finite-differences are somewhat more expensive and somewhat less accurate than rectangular FEs.

Products

Consider the problem of evaluating a product

$$v = uw, \tag{19}$$

where u and w are given at nodal points and we require values of v at these nodal points. Expanding as before in terms of the basis functions $e^i(x, y)$, multiplying by an arbitrary basis function $e^k(x, y)$ and orthogonalizing the error to the basis we obtain

$$\mathbf{P}\mathbf{v} = \mathbf{u}\mathbf{N}\mathbf{v}, \tag{20}$$

where \mathbf{P} is as before,

$$(\mathbf{u}\mathbf{N}\mathbf{v})_k = \sum_{i,j} u_i v_j \int_{\mathcal{D}} e^i(x, y) e^j(x, y) e^k(x, y) dx dy \tag{21}$$

the summations over i and j are performed over all nodal points, and \mathcal{D} is the domain.

The double sum in (21) is not as formidable as it appears since $e^k(x, y)$ is only non-zero in a relatively small neighbourhood of the k th node and therefore only nearest neighbours of u and v are involved in the calculation. Its efficient evaluation for rectangular (two-dimensional) and box (three-dimensional) elements is discussed in detail by Staniforth and Beaudoin¹¹ who show that it is advantageous to use Simpson quadrature rather than Gaussian. The evaluation of the right-hand side of (20) takes $O(MN)$ operations on an $M \times N$ grid for both rectangular and triangular elements (but triangular elements are more costly), and the prime difference in algorithmic efficiency is again the computational cost of solving a set of linear equations (the ‘mass-matrix problem’ $\mathbf{P}\mathbf{v} = \mathbf{R}$). For rectangular elements the solution of this problem is approximately a factor of two less expensive than the evaluation of the RHS but, as mentioned above, for triangular elements it is *considerably* more costly, both in terms of arithmetic operations and storage.

Additional economies possible with linear rectangular (and box) elements, and a useful notation

As a further illustration of efficiency ‘tricks’ that may be employed when using linear rectangular elements, consider the evaluation of

$$D = u_x + v_y, \tag{22}$$

where u, v and D are all functions of the three dimensions x, y and z . The Galerkin finite-element approximation to this equation may be written formally as

$$\mathbf{P}^x \mathbf{P}^y \mathbf{P}^z \mathbf{D} = \mathbf{P}_x \mathbf{P}^y \mathbf{P}^z \mathbf{u} + \mathbf{P}_y \mathbf{P}^x \mathbf{P}^z \mathbf{v}, \tag{23}$$

where \mathbf{P}^x and \mathbf{P}_x are tridiagonal one-dimensional operators having weights $(h_{m-1}/6, (h_{m-1} + h_m)/3, h_m/6)$ and $(-\frac{1}{2}, 0, \frac{1}{2})$, respectively, and with similar definitions obtaining for $\mathbf{P}^y, \mathbf{P}_y, \mathbf{P}^z$ and \mathbf{P}_z .

The solution of (23) is usually found by explicitly applying the six one-dimensional operators on the right-hand side and then successively ‘inverting’ the three one-dimensional operators on the left-hand side resulting in the successive application of nine operators of approximately equal cost. However we can achieve *exactly* the same result with half the work (i.e. by applying four operators instead of nine). To see this, we formally multiply (23) by $(\mathbf{P}^x)^{-1}(\mathbf{P}^y)^{-1}(\mathbf{P}^z)^{-1}$ and use commutativity of operators to obtain

$$\mathbf{D} = (\mathbf{P}^x)^{-1} \mathbf{P}_x \mathbf{u} + (\mathbf{P}^y)^{-1} \mathbf{P}_y \mathbf{v}.$$

These formal operations may be justified rigorously, and the end result is equivalent to using one-dimensional FEs along lines of constant y to calculate u_x , one-dimensional FEs along lines of constant x to calculate v_y , and then summing the result. Such a simplification is not possible with triangular (or tetrahedral) elements.

This is one example of the usefulness of the ‘subscript/superscript’ notation introduced above for rectangular (and box) elements. Another (similar) example is to consider the solution of the three-dimensional mass matrix problem $\mathbf{P}\mathbf{v} = \mathbf{r}$, where \mathbf{r} is given. Rewriting \mathbf{P} as the product $(\mathbf{P}^x\mathbf{P}^y\mathbf{P}^z)$ of one-dimensional operators, this problem reduces to the successive solution of three sets of one-dimensional problems, namely

- (i) solve $\mathbf{P}^z\mathbf{f} = \mathbf{r}$ for columns (fixed x and y)
- (ii) solve $\mathbf{P}^y\mathbf{g} = \mathbf{f}$ for fixed x and z
- (iii) solve $\mathbf{P}^x\mathbf{v} = \mathbf{g}$ for fixed y and z .

Again, the algorithm is of optimal order (i.e. $O(1)$ operations per node) and does not require any I/O to mass storage. Such a problem may, for example, be easily solved within memory on a 1 million word Cray 1-S for a $51 \times 51 \times 51$ mesh in 0.026 seconds.

Rectangular vs. triangular elements

Why are rectangular elements (and box elements in three-dimensions) in general more efficient? Because the underlying geometrical partitioning of the domain, together with the form of the basis functions, leads to matrices whose structure may be exploited. Although linear rectangular elements at first glance appear more expensive than triangular elements (they need four degrees of freedom to define them, rather than three), the fact that they are expressible as the *product* of one-dimensional elements leads to considerable economies in their manipulation. Not only are fewer operations and less memory required in general for rectangular elements than for triangular (tetrahedral) elements, they are also inherently more vectorizable (because they are well-ordered in memory and easily accessed), further enhancing efficiency.

3. ELEMENT ORDER, SPATIAL EVOLUTIONARY ERROR AND CODE MODULARITY

Having indicated in the previous section the high cost for even simple problems of linear triangular elements when compared to both linear rectangular elements and finite differences, we now restrict our attention to rectangular elements. The next question to address is ‘among rectangular elements, which ones are most suitable for fluid flow problems?’. Put another way, is there any virtue to using higher-order elements (i.e. piecewise polynomials of higher order) such as quadratic or cubic elements, rather than linear elements? The answer appears to be no for several reasons, many of which may be found in Reference 12 in which Cullen and Morton analysed the error associated with calculating an advection term such as $u \partial v / \partial x$ directly or calculating it as a two-stage process (compute the derivative, then the product) when using linear elements in the context of an evolutionary problem. They concluded that both methods asymptotically give an $O(h^4)$ estimate for the spatial evolutionary error but that the two-stage method has a smaller coefficient. From a coding point of view, the two-stage method is probably to be preferred, since all terms may be computed in a modular way using a set of ‘kernel’ subroutines that handle the fundamental operations of differences, products and the solution of linear equations involving the mass matrix \mathbf{P} .

It has been found that quadratic elements are generally (there may be some exceptions) less

accurate and more costly than linear elements, not to mention more complicated. Why are they less accurate? Because they have no super-convergence properties at nodes. What about cubic elements? They can have super-convergence properties but are much more expensive to work with per degree of freedom, boundary conditions are difficult to implement, program complexity is increased and, because of their higher order, there are more computational modes to worry about. The law of diminishing returns seems to apply.

4. STAGGERED, NON-STAGGERED AND MIXED-ORDER ELEMENTS AND THE FORM OF THE GOVERNING EQUATIONS

When formulating a fluid flow model, one often has to choose among several different forms of the governing equations. Furthermore, in the finite-element framework one is not restricted to using the same elements for all variables. Two possibilities come immediately to mind. First it is possible to use equal-order elements on a staggered grid (by analogy with staggered FD formulations). Secondly it is possible to use the same grid for all variables but to use mixed-order elements (i.e. expand some of the dependent variables in terms of one set of elements, and the others in terms of another set of elements of different order). In an ideal world one would expect that the choice of the form of the governing equations would be independent of the choice of element. In fact, we do not live in an ideal world and the two choices are intimately linked.

As a first example of how these two choices are linked, consider the shallow-water equations ((1)–(3)). Williams¹³ analysed various formulations for the FE solution of the linearized one-dimensional form of these equations using linear elements on both staggered and unstaggered meshes, where either velocity components or vorticity and divergence (as in the Introduction of the present study) were used as the momentum variables. His analysis indicates that to obtain good results with linear elements it is necessary to use either

- (i) velocity components as momentum variables, and stagger the nodal points for the free-surface height, or
- (ii) vorticity and divergence as momentum variables and no staggering,

and furthermore that using velocity components as momentum variables and no staggering propagates energy in the wrong direction and is likely to cause noise problems in a non-linear model. That the conclusions of this analysis also apply to higher dimensions and the non-linear equations is well supported by

- (i) the absence of noise problems reported by Staniforth and Mitchell,^{1,14} Cullen and Hall¹⁵ and Staniforth and Daley¹⁶ when using vorticity/divergence formulations and unstaggered elements
- (ii) the importance of introducing artificial smoothing to eliminate noise problems when using velocity components and unstaggered elements, reported by Cullen¹⁷
- (iii) the absence of noise reported by Hua and Thomasset¹⁸ when using velocity components and staggered elements
- (iv) the noise problems reported by Walters¹⁹ for some of the formulations examined.

Williams¹³ analysis is applicable to equal-order (namely linear) elements. It is also possible to use mixed-order elements (e.g. linear elements for velocity components and constant elements for free-surface height and vice versa), and it was concluded by Williams and Zienkiewicz²⁰ and Walters¹⁹ that such schemes are viable.

The above discussion is centred on horizontal considerations, but similar considerations should

also be expected to apply in the vertical. An analysis of a linearized version of the vertical FE discretization scheme of Staniforth and Daley²¹ for the hydrostatic primitive equations is given by Béland *et al.*²² The analysis is similar in concept to that of Williams,¹³ but focuses on the vertical instead of the horizontal. For the particular scheme analysed (unstaggered linear elements) it was shown that there is no spurious vertical propagation of energy in the wrong direction and that the scheme is basically sound. This analysis and that of Côté *et al.*²³ did however lead to the diagnosis of a weakness, namely the existence of a vertical computational mode.

Although this mode may in principle be forced by the parametrized terms of the model, in practice it was found that a small amount of vertical diffusion adequately controls it. The source of the weakness was traced (see equation 10.20 of Reference 23) to the form chosen for the governing equations, and in particular to the treatment of the hydrostatic equation. A revised formulation has been successfully implemented by Béland and Beaudoin.²⁴

Cliffe²⁵ presented an interesting analysis (based on the earlier analysis of Lee *et al.*²⁶) of the conservation properties of GFEM approximations to the Boussinesq equations. The basic idea is to expand each variable in terms of a finite-element space of unspecified order (or degree of continuity), and then to examine the conservation consequences of specific choices. An interesting feature of this framework is that it is easy to determine the *minimum* degree of continuity required of a certain variable after that of another has been set. The key point here is that if the finite-element space is too large (i.e. of too high an order) then computational modes will appear ('spurious pressure modes' in the terminology of Cliffe²⁵). It appears therefore to be desirable to choose the element order for one of the dependent variables of the problem (the higher the order, the higher the degree of complexity of the final algorithm), and to choose the minimum order for the other variables that is required to satisfy the desired conservation laws. Although the present author is not convinced that the best schemes are necessarily those which exactly conserve certain quantities (rather than those that almost conserve a larger number) the above-mentioned framework is nevertheless a valuable analysis tool for choosing elements appropriate to a given problem.

5. STABILITY

The stability properties of FE schemes turn out to be very similar to those of FD schemes. For pure advection (i.e. equation (3) with a non-divergent velocity field), a leap-frog scheme is conditionally stable whereas a forward (Euler) time scheme is unconditionally unstable.⁴ For pure diffusion, a leap-frog scheme is unconditionally unstable, whereas a forward scheme is conditionally stable. These conclusions hold true for both FD and FE schemes, and the principal differences in stability are that the coefficients appearing in the stability conditions are slightly different. For one-dimensional advection, for example, a leap-frog scheme using linear FEs has a stability condition $C = U \Delta t / \Delta x < 0.58$, whereas for centred second-order FDs $C < 1$, and for centred fourth-order FDs $C < 0.73$. Thus the most restrictive of these schemes from the point of view of stability is the FE one; however it is also the most accurate, and the price for increased accuracy is thus increased cost (i.e. more time steps).

A stability analysis of three different schemes (FD, FE and spectral) for solving the linearized shallow-water equations (cf. (1–3)) using a semi-implicit time scheme is given by Staniforth and Mitchell.¹ This analysis is performed in terms of response functions, and the conditions for stability for each of the three schemes is obtained by substituting the response functions appropriate to the method into the final result. The analysis was performed for a formulation using vorticity and divergence as momentum variables (cf.(1)–(3)) and also for two different formulations using velocity components as momentum variables. For an FE discretization it was concluded that one of the velocity component formulations was not viable because it was overdamped, the other was not

viable because it was computationally too expensive, and that this is a direct consequence of using a semi-implicit time discretization. This choice of time discretization turned out to be quite fortunate, because only the vorticity/divergence formulation was left, which Williams¹³ later demonstrated was the only FE scheme on an unstaggered grid using linear elements that does not suffer from propagation of small scales in the wrong direction!

A second example of a stability analysis is that given by Côté *et al.*²³ for the hydrostatic primitive equations. This analysis, although applied principally to the vertical discretization FE scheme of Staniforth and Daley,²¹ is also applicable to FD discretization schemes. It is similar to that described by Simmons *et al.*²⁷ its principal virtues being that it is somewhat more general and less empirical. An explicit stability criterion (that the static stability of the reference temperature profile be greater than the explicit one) is given in the limit of small Δt for a case examined numerically by Simmons *et al.*²⁷ and there is good agreement between the results. It was also shown that the first modes to go unstable if the criterion is violated are the computational modes due to the use of a (three time-level) semi-implicit time scheme. All of these conclusions apply equally well to FD schemes as they do to FE schemes, except for minor details. It seems in general that there are no further stability considerations to worry about, beyond those of FD schemes.

6. SOME FURTHER CONSIDERATIONS

Although finite-element Galerkin schemes are optimal in the sense that for a given choice of finite-element space they orthogonalize the error to the basis, this does not necessarily mean that in the context of a fluid flow model they are the optimum choice among algorithms of a given complexity. An illustration of this point may be found in Reference 1, where Staniforth and Mitchell showed that a minor change in the approximation of second derivative terms, and no changes elsewhere, led to a striking improvement in the accuracy of the results. To see why this is so, we examine the problem of evaluating second derivatives.

Second derivatives

Consider the problem of evaluating

$$v = u_{xx}, \tag{24}$$

where u is known at the set of nodal points, and we require values of v at these same points. Expanding u and v in terms of linear FEs (cf. equation (13)) and orthogonalizing the error to the basis (by multiplying by an arbitrary basis function $e^k(x)$ and integrating over the domain) we obtain

$$\mathbf{P}^x \mathbf{v} = \mathbf{P}_{xx} \mathbf{u}, \tag{25}$$

where \mathbf{P}^x and \mathbf{P}_{xx} are tridiagonal matrices having weights $[h_{m-1}/6, (h_{m-1} + h_m)/3, h_m/6]$ and $[1/h_{m-1}, -1/h_{m-1} - 1/h_m, 1/h_m]$, respectively. It is easily shown by Taylor series that this gives an $O(h^2)$ approximation to the second derivative on any uniform subdomain, which is no better than that obtained for half the computational effort using centred second-order FDs. However, by rewriting (25) as

$$\mathbf{P}^x \mathbf{v} = \mathbf{P}_{xx} \mathbf{u}, \tag{26}$$

where \mathbf{P}^x has been modified to be a tridiagonal matrix having weights $[h_{m-1}/12, 5(h_{m-1} + h_m)/12, h_m/12]$, we obtain an $O(h^4)$ approximation at no extra computational cost as our reward for

venturing outside the Galerkin FE framework. One possible explanation for this phenomenon is that we are looking in the wrong mathematical space when we use linear FEs to approximate second derivatives. Linear FEs only permit a ‘weak’ (in mathematical terminology) approximation to such derivatives because of a lack of continuity of derivatives in our choice of finite-element space; for these terms we should really be looking in a space having an added degree of continuity, but in practice it is more expedient to ‘bend’ the rules of the Galerkin FE method.

Staniforth and Mitchell¹ demonstrated that this idea does not adversely affect the computational stability of an FE fluid flow model (the shallow-water equations of section 1), and can be used to good advantage for problems in higher dimensions such as the solution of the two-dimensional Poisson problem

$$f_{xx} + f_{yy} = g. \quad (27)$$

The approximation used for this problem was

$$(\mathbf{P}^y \mathbf{P}_{xx} + \mathbf{P}^x \mathbf{P}_{yy})\mathbf{f} = \mathbf{P}^x \mathbf{P}^y \mathbf{g}, \quad (28)$$

where \mathbf{P}_{yy} and \mathbf{P}^y are the analogues of \mathbf{P}_{xx} and \mathbf{P}^x , as redefined above. The resulting set of difference equations (involving a nine-point operator) was solved using discrete Fourier transforms, which are economical in their memory requirements ($O(MN)$ on an $M \times N$ mesh) and computational effort ($O(MN \log N)$ operations).

Aliasing

Let us now turn our attention towards aliasing and compare the FE treatment with the FD treatment. It is well known that evaluating the pointwise product of the two terms involved in an advection term (such terms are implicitly contained in the RH sides of (1)–(3)) generally leads to non-linear computational instability in the context of an evolution problem. The cause of this instability is the aliasing of that part of the spectrum generated by the product that cannot be resolved by the mesh. The cure in all Eulerian methods (FD, FE, spectral, etc.) is to either implicitly or explicitly control this aliasing by smoothing (filtering) the result. The spectral method is the most direct and simply ignores the least significant half of the spectrum, whereas FD methods smooth by averaging various quantities.

The optimum treatment of aliasing is therefore a trade-off between accuracy and stability; too little smoothing leads to computational instability, whereas too much degrades accuracy. Where does the FE method stand in all this? An illuminating example is given by comparing Arakawa’s²⁸ approximation for two-dimensional incompressible flow on a uniform grid with that of the FE method using linear elements. It was shown by Jespersen²⁹ that the treatments of the advection terms are identical. The only difference between the two methods, therefore, is that the time derivative term in the FE approximation is multiplied by the projection (or mass) matrix \mathbf{P} of section 2, and the FE method is consequently a little more expensive. However the FE approximation leads to an $O(h^4)$ estimate for the spatial evolutionary error¹² rather than the $O(h^2)$ estimate for Arakawa’s²⁸ method, and the increased accuracy more than compensates for the added work.

Noting that the application to one side of an equation of a ‘smoothing’ operator (such as the projection matrix \mathbf{P}) is equivalent to the application to the other side of an ‘unsmoothing’ operator, the above result may be interpreted as follows: both methods control stability by using the same smoothing operator, but the FE method ‘sharpens the response’ to increase accuracy without adversely affecting stability, and is consequently a more efficient scheme.

Boundary conditions

An often-overlooked aspect of the FE method when using linear elements as compared to higher-order FD schemes, is the incorporation of boundary conditions. Higher-order FD schemes in the literature usually achieve better accuracy by involving more neighbouring points in the calculations, thus increasing the bandwidth of the matrices involved. For example, fourth order FD derivative approximations in one dimension involve five adjacent points rather than the three adjacent points of second-order FDs and the FE method using linear elements. In three-point schemes, the boundary conditions are used to obtain an equation associated with a boundary point, and the discretized governing equation is applied directly at all internal points. With a five-point FD scheme it is necessary to impose an extra computational boundary condition at all the internal points immediately adjacent to the boundary in order to obtain as many equations as there are unknowns. This can be a delicate procedure and if not done properly can result in the forcing of the computational modes associated with the use of a higher-order difference scheme. The linear FE scheme on the other hand can achieve fourth-order accuracy (for a first derivative, for example) without the need for additional (artificial) boundary conditions for the points immediately adjacent to boundaries. This is particularly advantageous when solving Poisson problems such as (10) and (11).

Mapping domains

The mapping of domains to a rectangle or box when using FE methods may be achieved in several ways. The most popular of these⁶ is to apply the FE method to the governing equations on a distorted mesh in physical space, and then evaluate the FE integrals after parametric transformation to a uniform mesh. These integrals contain the Jacobian of the transformation and are usually evaluated numerically by Gaussian quadrature, although this is not necessarily optimal.¹¹

An alternative approach, advocated by Srinivas and Fletcher,³⁰ is to first transform the governing equations from physical space to transformed space and then to apply the FE method to the transformed equations in transformed space. They argue that ‘... the resulting algorithm is both more accurate and more economical than applying the conventional finite-element method with an isoparametric mapping’. One disadvantage of this approach is a substantial increase in the number of terms in the governing equations after transformation (almost a tripling for their two-dimensional incompressible flow).

A transformation of the governing equations to another co-ordinate system gives rise in general to variable coefficients and cross-derivative terms. A particularly useful transformation in this regard is the *conformal transformation* (Reference 31, Chapter 7). It is a *global* transformation (as opposed to being *local* as in a parametric transformation), and has several useful properties. In particular, angles are invariant under transformation and the del squared operator retains its form, except that it is multiplied by a variable coefficient. Tables of useful conformal mappings may be found in References 31 and 32.

Flows that are conformally mappable to a rectangle include those in a periodic channel, around obstacles (e.g. aerofoils) in an unbounded domain, and within a rotating annulus. The polar-stereographic projection of the shallow-water equations over a sphere, given in the Introduction, is a further example of a conformally mapped flow; it is a particular case of the more general three-dimensional flow given by Staniforth and Daley.¹⁶ As can be seen from this last example, the governing equations do not become significantly more complicated after a conformal transformation. The accuracy of solutions in the physical domain is determined by the accuracy of the solution in the transformed domain, and the solutions will be accurate provided strong gradients in the transformed domain are well resolved and the transformation is reasonably smooth.

7. TIME SCHEMES

The choice of time discretization and how it interacts with the space discretization can have an important impact on the efficiency of a fluid dynamics code. The simplest time schemes are explicit. In these schemes the partial time derivative of a variable is isolated on the left-hand side of an equation and approximated in terms of a time difference involving the new and previous time steps, whereas the right-hand side is evaluated explicitly using known values of the dependent variables at previous time steps. The right-hand side may be evaluated using the traditional Galerkin FE method,⁶ by breaking it down into several steps¹² or by grouping them together as fluxes (the 'group FE method' of Fletcher⁷). Terms on the right-hand side are evaluated using the methods described in the preceding sections, and the mass matrix problem (associated with the time differencing of the left-hand side) is solved using the efficient algorithm of section 2.

Explicit time schemes are very efficient and appropriate for problems where the time step is restricted by the time truncation error rather than by stability considerations. However, they are not particularly efficient for stiff sets of equations (such as the shallow-water equations (1)–(3)), and it is often advantageous to treat some, or all, of the terms implicitly in time. This can be done in several ways. Baker and Soliman,⁶ for example, approximate all terms as time averages or differences over times $n\Delta t$ and $(n+1)\Delta t$. This results in a set of coupled non-linear equations at each time step which are solved iteratively. The advantage of such an approach is that fewer time steps are required for stiff systems of equations because of the enhanced stability. The disadvantage is that each time step is more costly than that of an explicit time scheme because of the need to iterate. Nevertheless this approach can be cost effective, provided that the time step may be increased significantly without loss of accuracy, and the iterative technique is efficient. Baker and Soliman⁶ ensure that the operator on the left-hand side is expressible as the tensor product of one-dimensional operators, which makes each iteration highly efficient.

A related alternative is the family of alternating-direction implicit schemes such as those of Srinivas and Fletcher³⁰ and Cohn *et al.*³³ Here, terms of $O(\Delta t^2)$ at the new time step are added to a linearized time discretization of the equations in such a way as to obtain tensor product operators similar to those of Baker and Soliman.⁶ The principal difference in the definition of the tensor product operators of the schemes is that those of Srinivas and Fletcher³⁰ and Cohn *et al.*³³ are linear (and the linear matrix problem is solved explicitly), whereas that of Baker and Soliman⁶ is non-linear (and the non-linear matrix problem is solved iteratively). The alternating-direction implicit (factored) methods also have enhanced stability properties with larger time steps and have the advantage of requiring less computational effort per time step than the fully implicit scheme of Baker and Soliman.⁶ The disadvantage of the alternating-direction implicit methods is that although they are stable with large time steps they are unfortunately not necessarily accurate. This has been shown by Yakimiw and Robert³⁴ to be the case for the discretization by Cohn *et al.*³³ of the shallow-water equations.

A further alternative, particularly effective for stiff sets of equations, is to identify those terms that are responsible for restricting the time step because of stability. The linear contributions of these terms are then treated implicitly in time, whereas perturbations about them, and the remaining terms, are treated explicitly. This idea was first applied to a finite-difference discretization of the shallow-water equations by Kwizak and Robert,³⁵ who found that such a scheme (which they termed semi-implicit) is five times more efficient than an explicit leap-frog scheme. Later, Staniforth and Mitchell^{1,14} applied it to an FE discretization of the same equations with a similar improvement.

The extension to the three-dimensional hydrostatic primitive equations was first demonstrated for an FD discretization by Robert *et al.*³⁶ and subsequently by Staniforth and Daley¹⁶ for an FE

formulation. The hydrostatic primitive equations are a set of three-dimensional dynamic equations that govern (at least to leading order) the flow of the atmosphere. They include the horizontal momentum equations, the equation of continuity (including compressible effects), the thermodynamic equation, an equation of state and the hydrostatic equation. This last equation replaces the vertical momentum equation, and consists of its two most important terms, which are in approximate balance and several orders of magnitude larger than the neglected ones.

Semi-implicit schemes offer a good compromise for stiff systems of equations. They require fewer time steps than explicit schemes (because of their enhanced stability) and yet do not require significantly more computations per time step.

8. CONCLUSIONS—OPTIMAL (?) SCHEMES

For fluid flow problems in regular domains, it appears at this time that triangular (and tetrahedral) elements cannot in general compete with rectangular (and box) elements, because they do not permit an efficient solution of the mass-matrix problem. An optimal (or close to optimal) scheme for given computational effort in this context is most likely to be achieved by a judicious mix of techniques.

First derivative and product terms seem to be well handled by GFEM schemes using linear rectangular (and box) elements. They have the attributes of simplicity, accuracy stability and straightforward incorporation of boundary conditions, and compete favourably with fourth order FD schemes. However for these elements it is often advantageous to go outside the Galerkin framework when approximating second derivatives, as described in section 6. Higher-order rectangular elements are a possibility, but the introduction of more computational modes and added programming complexity are decided disadvantages, and the law of diminishing returns would seem to apply.

It is important to analyse carefully the properties of linearized versions of the discrete models in order to obtain maximum accuracy and efficiency. Of particular importance is the form of the governing equations, *vis-à-vis* the choice of staggered, non-staggered and/or mixed-order elements, and the choice of an appropriate time scheme.

In conclusion, the described techniques have been successfully applied to a variety of problems in regular domains, such as the three-dimensional time-dependent hydrostatic primitive equations; these are stiff and include first and second derivative terms, non-linearities, and variable coefficients due to a conformal mapping.

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