AN IMPROVED METHOD FOR INTEGRATING THE MIXED SPECTRAL FINITE DIFFERENCE (MSFD) MODEL EQUATIONS

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Abstract. In their Mixed Spectral Finite Difference (MSFD) model for flow over complex terrain, Beljaars *et al.* (1987) solve a set of coupled, second-order ordinary differential equations (ODEs) for the first-order perturbations to the logarithmic velocity profile caused by nonuniform surface roughness and topography. To solve this set of ODEs, they employ a Forward Euler Shooting Method. It is demonstrated here that the shooting method is computationally unstable for this problem. An absolutely stable finite-difference method based on a block tridiagonal LU factorization of the finite-difference matrix is presented. The advantages of the present algorithm over the method used by Beljaars *et al.* are demonstrated both by theoretical argument and numerical experiment.

1. Introduction

In a recent paper, Beljaars *et al.* (1987), hereafter referred to as BWT, present a linear *M*ixed *S*pectral *F*inite *D*ifference (MSFD) model for neutral surface-layer flow over complex terrain. They employ a Forward Euler Shooting Method to solve equations for the first-order perturbation to the flow caused by topography and by variations in surface roughness. In a comparison with measured field data, the algebraic stress version of their model is seen to make good predictions of both the mean flow and turbulent stresses (BWT, Section 5). However, the numerical method employed exhibits divergent behaviour under certain conditions. In this paper, a significantly more robust and accurate numerical method is presented.

2. The MSFD Model Equations

In the interest of brevity, the model equations will be presented here with minimal detail. For a more exhaustive discussion that includes the rationale for model approximations, the reader is referred to BWT.

In formulating their model, BWT begin with the Reynolds-averaged stationary Navier–Stokes equations in Cartesian coordinates (BWT, Equation (1)). They transform to an (x, y, Z) coordinate system where the Z-coordinate is terrain-following:

$$Z = z - f_1(x, y), \tag{1}$$

where $f_1(x, y)$ is the height of the surface above a reference level.

To make the problem tractable, BWT postulate that the solution to the nonlinear

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model equations can reasonably be decomposed into the sum of a zero-order solution for horizontally homogeneous flow over a flat surface of uniform roughness, z_0, and small first-order corrections that account for variations in topography and surface roughness (BWT, Equations (3), (3a), and (4)). This approximation reduces the original nonlinear problem to the solution of a set of coupled, linear partial differential equations for the first-order perturbations. The solution of this set of equations is realized by first performing a finite-area Fourier transform in the $x - y$ plane. For the wavenumber pair (k, m), this operation yields the following set of coupled ordinary differential equations:

$$iu_{op}(Z)\hat{u}_1 + \frac{\mathrm{d}u_0}{\mathrm{d}Z}\,\hat{w}_1 = -\frac{1}{\rho}\,ik\hat{p}_1 + \frac{\partial}{\partial Z}\,\hat{\tau}_{x1}\,,$$

$$iu_{op}(Z)\hat{v}_1 + \frac{\mathrm{d}v_0}{\mathrm{d}Z}\,\hat{w}_1 = -\frac{1}{\rho}\,im\hat{p}_1 + \frac{\partial}{\partial Z}\,\hat{\tau}_{y1}\,,$$

$$iu_{op}(Z)\hat{w}_1 - u_{op}^2(Z)\,\hat{f}_1 = -\frac{1}{\rho}\,\frac{\partial}{\partial Z}\,\hat{p}_1\,,$$

$$ik\hat{u}_1 + im\hat{v}_1 + \frac{\partial}{\partial Z}\,\hat{w}_1 = 0\,, \tag{2}$$

where

$$u_{op}(Z) = ku_0(Z) + mv_0(Z)\,,$$

$$u_0(Z) = \frac{\cos\phi}{\kappa}\,\ln[(Z + z_0)/z_0]\,,$$

$$v_0(Z) = \frac{\sin\phi}{\kappa}\,\ln[(Z + z_0)/z_0]$$

and the 'top-hat' symbol denotes Fourier-transformed quantities. All symbols have the meaning attached to them in BWT except that velocities (and stresses) have been normalized by the friction velocity, u_*, corresponding to the zero-order velocity profile.

BWT study several alternative closure schemes including the mixing-length hypothesis, an $E - \varepsilon$ model and an algebraic stress closure. All three closure schemes make similar predictions for mean flow quantities; however, the mixing-length hypothesis was found to be inferior to the $E - \varepsilon$ and algebraic stress models for predictions of surface stresses. Furthermore, in the outer layer, stresses predicted by the algebraic stress model are more realistic than those calculated from the $E - \varepsilon$ model. Considering the superiority of the algebraic stress closure over other closures, this paper will focus on that version of their model.

In the algebraic stress model employed by BWT, the first-order perturbations to the

turbulent shear stresses are calculated according to

$$\hat{\tau}_{x1} = \frac{\kappa(Z + z_0) \dfrac{\partial}{\partial Z} \hat{u}_1 + \cos(\phi)\,[2\alpha\hat{E}_1 - \hat{\psi}_1]}{1 + i \dfrac{\kappa(Z + z_0)}{C_3} u_{op}(Z)}$$

$$\hat{\tau}_{y1} = \frac{\kappa(Z + z_0) \dfrac{\partial}{\partial Z} \hat{v}_1 + \sin(\phi)\,[2\alpha\hat{E}_1 - \hat{\psi}_1]}{1 + i \dfrac{\kappa(Z + z_0)}{C_3} u_{op}(Z)} \tag{3}$$

where $\hat{E}_1$ is the Fourier transform of the first-order pertubation to the turbulent kinetic energy and $\hat{\psi}_1$ is related to the Fourier transform of the first-order perturbation to the dissipation, $\hat{\varepsilon}_1$, by the relation

$$\hat{\psi}_1 = \hat{\varepsilon}_1(Z + z_0) \tag{4}$$

The first-order perturbation to the turbulent kinetic energy is required to satisfy

$$iu_{op}(Z)\hat{E}_1 = \frac{2}{\kappa(Z + z_0)} (-\alpha\hat{E}_1 + \hat{\tau}_{x1}\cos(\phi) + \hat{\tau}_{y1}\sin(\phi)) +$$

$$+ \frac{\partial}{\partial Z}\left(\frac{\kappa(Z + z_0)}{C_{KE}} \frac{\partial}{\partial Z} \hat{E}_1\right) \tag{5}$$

and the quantity $\hat{\psi}_1$ is calculated from

$$iu_{op}(Z)\hat{\psi}_1 = \frac{1}{(Z + z_0)} \hat{w}_1 + \frac{2\alpha(C_{\varepsilon 1} - C_{\varepsilon 2})}{\kappa(Z + z_0)} \hat{\psi}_1 -$$

$$- (3C_{\varepsilon 1} - C_{\varepsilon 2}) \frac{\alpha^2}{\kappa(Z + z_0)} \hat{E}_1 +$$

$$+ C_{\varepsilon 1} \frac{2\alpha}{\kappa(Z + z_0)} (\hat{\tau}_{x1}\cos(\phi) + \hat{\tau}_{y1}\sin(\phi)) +$$

$$+ \frac{\kappa(Z + z_0)}{C_{K\varepsilon}} \frac{\partial}{\partial Z}\left(\frac{\partial}{\partial Z} \hat{\psi}_1 - \frac{2\alpha}{Z + z_0} \hat{E}_1\right). \tag{6}$$

Given that in the near-surface zone, the solution is approximately logarithmic and in the outer layer it is very nearly exponential, BWT employ the coordinate transformation

$$\eta = \frac{\ln[(Z + z_0)/z_0]}{\ln[(l_i + z_0)/z_0]} + Z/l_0\,, \tag{7}$$

where l_i and l_o are the inner and outer length scales, respectively. Following the theory of Hunt and Simpson (1982), the length scales l_i and l_o are chosen to be wavenumber-dependent.

$$(l_i/L)\ln(l_i/z_o) = 2\kappa^2\,, \tag{8a}$$

$$l_o = (k^2 + m^2)^{-1/2}\,. \tag{8b}$$

In Equation (8a) above, L is the horizontal scale of the perturbation (topography or roughness induced) and is calculated according to Equation (9).

$$L = |k\cos\phi + m\sin\phi|^{-1}\,. \tag{9}$$

Equations (8) and (9) are inappropriate for highly anisotropic perturbations (for example, when $m \gg k$). In the highly anisotropic case for certain angles ϕ, the inner length scale l_i can exceed the outer length scale l_o. In these degenerate cases, an alternative definition for the inner and outer length scales must be employed.

To solve Equations (2), (3), (5), and (6), boundary conditions are required both at the surface and at some as of yet unspecified upper boundary. Near the surface (i.e., in the vicinity of $\eta = 0$), it is assumed that a shallow, constant-stress wall layer exists within which $\hat{u}$ and $\hat{v}$ satisfy the following relations:

$$\hat{u}_1 = \left[\frac{\hat{\tau}_{x1}}{\kappa} - \frac{\cos\phi}{2\kappa}\,(\hat{\tau}_{x1}\cos\phi + \hat{\tau}_{y1}\sin\phi)\right]\ln\frac{Z + z_0}{z_0} + \frac{\cos\phi}{\kappa}\,\hat{m}_1\,,$$

$$\hat{v}_1 = \left[\frac{\hat{\tau}_{y1}}{\kappa} - \frac{\sin\phi}{2\kappa}\,(\hat{\tau}_{x1}\cos\phi + \hat{\tau}_{y1}\sin\phi)\right]\ln\frac{Z + z_0}{z_0} + \frac{\sin\phi}{\kappa}\,\hat{m}_1\,, \tag{10}$$

where $\hat{m}_1$ is the Fourier transform of the function $m_1(x, y)$ which relates the local roughness length, z_{01}, to the upstream roughness length z_0 by

$$z_{01}(x, y) = z_0\, e^{-m_1(x,y)}\,. \tag{11}$$

Additionally, at $\eta = 0$, we must have

$$\hat{w}_1 = 0\,. \tag{12}$$

BWT require $\partial\hat{E}_1/\partial Z$ and $\partial\hat{\psi}_1/\partial Z$ to vanish at $\eta = 0$. We prefer to employ a local equilibrium hypothesis to deduce boundary conditions on $\hat{E}_1$ and $\hat{\psi}_1$. If it is assumed that production and dissipation of turbulence are in local equilibrium in a thin wall layer, then $\hat{E}_1$ and $\hat{\psi}_1$ must satisfy

$$\alpha\hat{E}_1 = \hat{\tau}_{x1}\cos\phi + \hat{\tau}_{y1}\sin\phi\,, \qquad \hat{\psi}_1 = \tfrac{3}{2}\alpha\hat{E}_1\,. \tag{13}$$

Beljaars (1985) has demonstrated that at heights several times the local roughness length, differences between the zero gradient and equilibrium boundary conditions are negligible.

Ideally, the upper boundary conditions should be imposed at infinity where perturbations to the flow are known to vanish. However, in practice, the upper boundary

conditions are imposed at a height $\eta = \eta_b$, where η_b is chosen to equal a large but finite number. To derive boundary conditions at $\eta = \eta_b$, the flow above η_b is assumed to be inviscid and irrotational. It follows from this approximation that at $\eta = \eta_b$,

$$p_1 = \frac{iu_{op}}{\alpha_k}\,\hat{w}_1 - \frac{u_{op}^2}{\alpha_k}\,\hat{f}_1\,, \tag{14a}$$

$$\hat{\tau}_{x1} = \frac{-\dfrac{\cos\phi}{Z+z_0}\,\hat{f}_1 + \dfrac{k\alpha_k\kappa(Z+z_0)}{u_{op}}\,\hat{p}_1}{1 + \kappa u_{op}(Z+z_0)/C_3} \tag{14b}$$

and

$$\hat{\tau}_{y1} = \frac{-\dfrac{\sin\phi}{Z+z_0}\,\hat{f}_1 + \dfrac{k\alpha_k\kappa(Z+z_0)}{u_{op}}\,\hat{p}_1}{1 + \kappa u_{op}(Z+z_0)/C_3} \tag{14c}$$

where $\alpha_k = (k^2 + m^2)^{-1/2}$. Furthermore, at the upper boundary, perturbations to the turbulent kinetic energy and the dissipation are required to vanish.

To solve the model equations, BWT employ a first-order accurate shooting method. Beljaars (1985) reports, however, that for large values of λ/z_0, where

$$\lambda = \frac{2\pi}{(k^2 + m^2)^{1/2}}\,, \tag{15}$$

the shooting method is unstable. This problem did not develop for the mixing-length closure, but was prominent for the $E - \varepsilon$ and algebraic stress closures. The problem is exacerbated for large η_b; consequently Beljaars performed some of his calculations using a different definition for l_o than that given above, namely

$$l_o = 10 l_i\,. \tag{16}$$

Although η_b was left unchanged, redefining l_o according to (16) effectively lowered the height of the upper boundary. In certain cases, this action might be undesirable. In the next section, an analysis of the instability encountered by Beljaars is presented and an alternative to the shooting method is proposed that is unconditionally stable for any choice of λ/z_0 or η_b.

3. Numerical Analysis of the MSFD Equations

3.1. The shooting method

Rather than applying a two-point boundary-value finite-difference technique to the MSFD model equations, BWT employ a forward Euler shooting method. There are at least two good reasons for choosing the shooting method over a finite difference

formulation. First, the shooting method is very easy to code. Second, the shooting method is computationally economical. For the solution of a set of q coupled first-order ordinary differential equations at N levels by the shooting method, $\mathcal{O}(Nq^2)$ floating point operations are required. Using a corresponding finite-difference method, $\mathcal{O}(Nq^3)$ operations are required if the block tridiagonal structure of the difference equation is exploited and the operation count rises to $\mathcal{O}(N^3q^3)$ if the difference matrix is treated as though it is full. Despite these advantages, the shooting method should be cautiously applied to boundary-value problems because parasitic solutions can cause the method to be computationally unstable.

Following the standard shooting method for boundary-value problems, the MSFD model equation set, Equations (2) through (6) inclusive, can be recast as an initial-value problem:

$$\frac{\partial}{\partial Z}\,\Phi = F(\Phi,\ Z;\ k, m, z_0,\ \hat{f}_1, \hat{m}_1)\,, \tag{17}$$

where

$$\Phi = \left[\hat{w}_1,\ \hat{\tau}_{x1},\ \hat{\tau}_{y1}, \hat{E}_1,\ \hat{\psi}_1,\ \hat{p}_1, \hat{u}_1,\ \hat{v}_1,\ \frac{\kappa(Z+z_0)}{C_{K\varepsilon}}\ \partial\hat{E}_1/\partial Z,\ \partial\hat{\psi}_1/\partial Z\right]^T$$

with initial conditions

$$\tilde{\alpha}\,\Phi + \tilde{\beta}\ \frac{\partial}{\partial Z}\,\Phi = \gamma\,, \tag{18}$$

where $\tilde{\alpha}$ and $\tilde{\beta}$ are 10×10 matrices and γ is a vector. Note, however, that $\tilde{\alpha}$, $\tilde{\beta}$, and γ are not fully specified and must be determined as part of the solution process.

Since F is linear in Φ, $\hat{m}_1$, and $\hat{f}_1$, BWT consider the roughness and topographic perturbations separately. They decompose Φ into the sum $\Phi = \Phi_r + \Phi_t$, where Φ_r and Φ_t are the roughness and topographic perturbations, respectively. Φ_r and Φ_t satisfy

$$\frac{\partial}{\partial Z}\,\Phi_r = (\Phi_r,\ Z;\ k, m, z_0,\ \hat{f}_1, 0)\,,$$

$$\frac{\partial}{\partial Z}\,\Phi_t = (\Phi_t,\ Z;\ k, m, z_0, 0, \hat{m}_1)\,, \tag{19}$$

with initial conditions like those of Equation (18).

The solution procedure employed by BWT has two steps:

(1) Subject to essentially arbitrary initial conditions, they repeatedly integrate Equation (18) from $\eta = 0$ to $\eta = \eta_b$ so as to generate five independent solutions to the homogeneous equations (i.e., $\hat{m}_1 = \hat{f}_1 = 0$) and two particular solutions ($\hat{m}_1 = 1$, $\hat{f}_1 = 0$ and $\hat{m}_1 = 0$, $\hat{f}_1 = 1$). The integration is accomplished by a fixed-step length

forward Euler method. In matrix notation, the Euler method can be represented as

$$A\Phi^{i+1} = B\Phi^i + b\,, \tag{20}$$

where i is an index that denotes the integration level. The matrix A is lower triangular and of dimension 10×10. Since A is lower triangular, Φ^{i+1} can be calculated explicitly from Φ^i.

(2) Let $\{\Phi_j^N \mid j = 1, 2, \ldots, 5\}$, Φ_m^N, and Φ_f^N be the homogeneous solution set, the particular solution for the roughness perturbation and the particular solution for the topography, respectively, at the upper boundary ($i = N$). The solution to the two-point boundary-value problem can be written

$$\Phi_r = \sum_{j=1}^{5} a_j^r \Phi_j + \Phi_m\,, \qquad \Phi_t = \sum_{j=1}^{5} a_j^t \Phi_j + \Phi_f\,. \tag{21}$$

To determine $\{a_j^r \mid j = 1, 5\}$ and $\{a_j^t \mid j = 1, 5\}$, Φ_r and Φ_t are required to satisfy (14); this involves the solution of two 5×5 systems of equations:

$$\mathcal{L}a^r = b^r\,, \qquad \mathcal{L}a^t = b^t\,. \tag{22}$$

Once a^r and a^t are known, the solution is fully determined.

Unfortunately, the procedure outlined above is computationally ill-conditioned. In Figure 1, the modulus of the residual on the stress pressure-relation (Equation (14b)) at $\eta = \eta_b$ normalized by the modulus of surface value of $\hat{\tau}_{x1}$ (which we shall call the relative error) is plotted against $\lambda/z_0 = 2\pi/(kz_0)$ for a two-dimensional sinusoidally varying perturbation of unit amplitude to the logarithm of the surface roughness length for the case $\phi = 0$ and $\eta_b = 3$. When λ/z_0 is small, the relative error is clearly negligible; however, by the time λ/z_0 exceeds 5×10^5, the relative error is no longer small and cannot be ignored. A similar pattern of error is to be found for all the components of Φ for both roughness and topographic perturbations. As a further example, the relative error in the perturbation to the turbulent kinetic energy at $\eta = \eta_b$ for a sinusoidal topographic perturbation of unit amplitude is plotted on the same figure.

For larger values of η_b, the computational instability is more acute. In Table I, the relative error in the stress-pressure relation (Equation (14b)) at the upper boundary (i.e., at $\eta = \eta_b$) for the aforementioned roughness perturbation with $\lambda/z_0 = 10^5$ is tabulated as a function of η_b. The relative error is seen to grow monotonically with η_b. For $\eta_b = 12$, the algorithm diverges.

There are two independent sources of the observed computational instability. First, the Forward Euler integration (Equation (20)) employed to calculate the set of independent solutions is unconditionally unstable – that is, for all values of λ/z_0, N, and η_b, round-off and truncation errors are amplified on passing from level i to $i + 1$. For (20) to be stable to round-off and truncation errors, it is necessary and sufficient that the spectral radius of $A^{-1}B$ (i.e., $\|A^{-1}B\|_2$) be less than or equal to one. In Table II, for $\eta_b = 3$ and various values of N, the geometric mean and minimum value of $\|A^{-1}B\|_2$ over all levels i, is tabulated. We see that the spectral radius of $A^{-1}B$ always exceeds

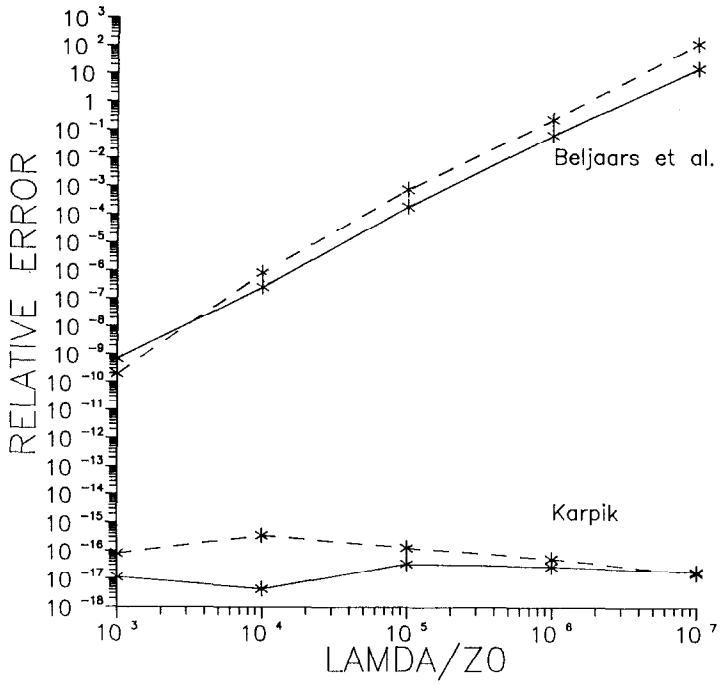

Fig. 1. Relative error in the stress-pressure boundary condition, Equation (14b), for a sinusoidal variation in surface roughness (dashed line) and relative error on the turbulent kinetic energy boundary condition, $\hat{E}_1 = 0$, for a sinusoidal topographic perturbation (solid line). For both the roughness and topographic perturbations, the upper boundary was located at $\eta_b = 3$. Computations were performed on a Cray 1-S computer using single-precision arithmetic (15 digit word length).

TABLE I

Relative error in $\hat{\tau}_{x1}$ at $\eta = \eta_b$ (roughness perturbation) for $\lambda/z_0 = 10^5$ and $\Delta\eta = 0.075$

η_b	Relative error
1.5	8.36×10^{-9}
3.0	7.73×10^{-4}
6.0	5.18×10^{1}
12.0	Diverges

unity. Further, we can deduce from the tabulated values that the spectral radius only asymptotically approaches unity in the limit as N tends to infinity.

A second cause of the observed computational instability in the shooting method is to be found at the stage where the coefficients $\{a_j^r \mid j = 1, 5\}$ and $\{a_j^t \mid j = 1, 5\}$ are calculated (Equation (22)). For large values of λ/z_0 (say, in the range 10^5 to 10^7 when $\eta_b = 3$), the matrix that must be solved to determine $\{a_j^r \mid j = 1, 5\}$ and $\{a_j^t \mid j = 1, 5\}$ is

TABLE II

Spectral radius of the matrix $A^{-1}B$ for $\eta_b = 3$

N	$\lambda/z_0 = 10^3$		$\lambda/z_0 = 10^5$		$\lambda/z_0 = 10^7$	
	Minimum	Mean	Minimum	Mean	Minimum	Mean
21	1.58	1.89	2.49	5.57	4.11	22.05
41	1.25	1.38	1.60	2.45	2.11	7.07
81	1.12	1.18	1.27	1.61	1.46	3.29
161	1.06	1.08	1.13	1.28	1.21	1.94

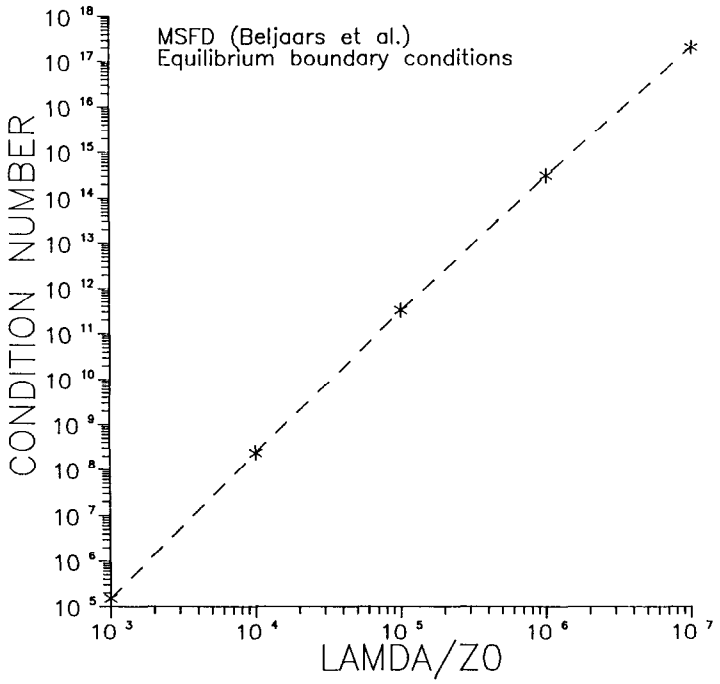

Fig. 2. Condition number of the matrix $\mathscr{L}$ as a function of λ/z_0.

poorly conditioned. In Figure 2, the condition number of the matrix $\mathscr{L}$ is plotted as a function of λ/z_0 for $\eta_b = 3$ and $N = 41$. If the condition number of the matrix $\mathscr{L}$ equals 10^n, then on a computer with a p digit word length, the solution vectors a^r and a^t will be accurate to only $(p - n)$ decimals. Therefore, even if we were to replace the Forward Euler integration with an A stable scheme (Gear, 1971), the poor conditioning of the matrix $\mathscr{L}$ would still render the shooting method unstable. A finite-difference formulation based on a block tridiagonal LU factorization of the MSFD model is proposed in the next section as a replacement for the shooting method.

3.2. A BLOCK LU FACTORIZATION FORMULATION

After central conservative differencing of the MSFD model equations, Equations (2)–(6), on a 'MAC-like' staggered grid (Harlow and Welch, 1965), we are left with the following system of difference equations:

$$\begin{aligned} &B_1\Phi_1 + C_1\Phi_2 = b_1\,, \\ &A_i\Phi_{i-1} + B_i\Phi_i + C_i\Phi_{i+1} = b_i\,, \qquad i = 1, 2, \ldots, N-1\,. \\ &A_N\Phi_{N-1} + B_N\Phi_N = b_N\,, \end{aligned} \tag{23}$$

Incorporated into (23) are the boundary conditions, Equations (10)–(14), at both $\eta = 0$ and $\eta = \eta_b$.

To derive a solution algorithm for the set of equations just above, it is preferable to recast (23) in matrix notation as follows:

$$\mathbb{A}\Phi = b\,, \tag{24}$$

where

$$\mathbb{A} = \begin{bmatrix} B_1 & C_1 & & & \\ A_2 & B_2 & C_2 & & \\ & A_3 & B_3 & C_3 & \\ & & \cdots\cdots\cdots\cdots & & \\ & & & A_N & B_N \end{bmatrix}$$

and $b = [b_1, b_2, \ldots, b_N]^T$. A_i, B_i, C_i are 8×8 matrices and Φ is as defined in Equation (17). The matrix $\mathbb{A}$ is said to be block triadiagonal. In direct analogy to the Thomas tridiagonal algorithm (Marchuk, 1982, pp. 212–223) for scalar tridiagonal systems of equations, a block variant of that algorithm can be derived.

Let it be assumed that the matrix $\mathbb{A}$ can be factored into the product form

$$\mathbb{A} = LU\,, \tag{25}$$

where

$$L = \begin{bmatrix} I & & & \\ L_2 & I & & \\ & L_3 & I & \\ & & \cdots\cdots & \\ & & L_N & I \end{bmatrix} \tag{26}$$

and

$$U = \begin{bmatrix} U_1 & C_1 & & & \\ & U_2 & C_2 & & \\ & & U_3 & C_3 & \\ & & \cdots & \cdots & \\ & & & & U_N \end{bmatrix}. \tag{27}$$

Once the matrix $\mathbb{A}$ has been factored as indicated above, a combined forward/backward sweep of the factored system efficiently yields the solution vector Φ. It remains, however, to specify first the matrices L_i and U_i in terms of known quantities. Recursion relations for L_i and U_i are easily derived by substituting for L and U from Equations (26) and (27) into (24) and comparing coefficients. Following this procedure it is deduced that

$$\begin{aligned} U_1 &= B_1 , \\ L_i &= A_i U_{i-1}^{-1} , \qquad i = 2, 3, \ldots, N . \\ U_i &= B_i - L_i C_{i-1} , \end{aligned} \tag{28}$$

It is not hard to see that for a block size of q ($q = 8$ for the MSFD algebraic stress model), the block tridiagonal algorithm can be realized at a cost of $\mathcal{O}(Nq^3)$ floating point operations. Gaussian elimination on the other hand would require $\mathcal{O}(N^3 q^3)$ operations to solve the same system of equations. For typical values of N in the neighbourhood of 40, the advantage of the block tridiagonal algorithm over full Gaussian elimination is considerable. Theoretically, we would expect the block tridiagonal algorithm to be about q times as expensive as the shooting method; this estimate is borne out by numerical experiments.

Varah (1972) has determined necessary and sufficient conditions which state requirements on the matrices A_i, B_i, and C_i so as to guarantee that the set of recursion relations stated in Equation (28) is numerically stable against the growth of round-off errors. It can be shown that for any reasonable discretization of Equations (2)–(6), the matrices A_i, B_i, and C_i satisfy Varah's stability conditions; therefore, the block tridiagonal algorithm represents an unconditionally stable solution technique for the MSFD model equations.

4. Example Calculations

For the extra cost involved in the block tridiagonal factorization, a considerable gain in accuracy and stability is realized. In Figure 1, previously referred to in the discussion of the shooting method, the relative errors in the upper boundary conditions for stress and turbulent kinetic energy as a function of λ/z_0 are plotted for both the shooting method and the block tridiagonal formulation. The latter formulation is several orders

of magnitude more accurate than the former even for low values of λ/z_0. Furthermore, the relative error of the block tridiagonal formulation is approximately constant over the range of calculated λ/z_0 values.

For a set of ordinary differential equations with constant coefficients, we would expect a central conservative difference scheme to be of second-order accuracy – it cannot be assumed without question that such a scheme would be of second-order accuracy when applied to the MSFD model equations which have non-constant coefficients. A grid refinement study conducted by the author demonstrated that the conservative central differences are in fact of order $\Delta\eta^2$ accurate. For $\eta_b = 3$, it is sufficient to use 41 vertical levels to achieve an accuracy of within 1% in the surface stress for $\lambda/z_0 = 10^5$.

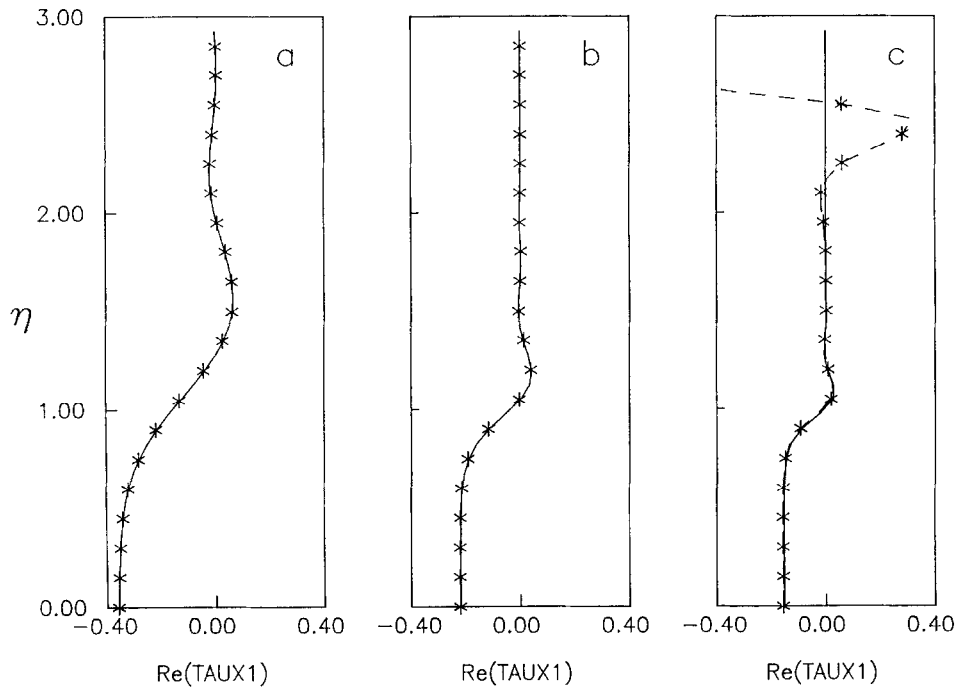

Fig. 3. Vertical profile of Re($\hat{\tau}_{x1}$) for a sinusoidal variation in surface roughness for (a) $\lambda/z_0 = 10^3$, (b) $\lambda/z_0 = 10^5$, and (c) $\lambda/z_0 = 10^7$. Calculations made with 41 vertical levels. (Karpik – solid line; Beljaars *et al.* – asterisks.)

In Figure 3, the real part of $\hat{\tau}_{x1}$ (corresponding to values above roughness maxima) for a two-dimensional sinusoidal variation of unit amplitude in the logarithm of the surface roughness length as calculated by both the shooting method and the block tridiagonal formulation, is plotted as a function of the vertical grid coordinate, η, for $\lambda/z_0 = 10^3$, 10^5, and 10^7, respectively. For $\lambda/z_0 = 10^3$, any differences between the two sets of calculations are imperceptible; when $\lambda/z_0 = 10^5$, there are some small but

noticeable differences between the results produced by the shooting method and the block tridiagonal formulation. The shooting method is obviously unstable for λ/z_0 equal to 10^7 whereas the block tridiagonal formulation continues to perform well. Similar results for a sinusoidal topographic perturbation of unit amplitude are presented in Figure 4. Again, differences between the stress profiles calculated by the two solution techniques are negligible for $\lambda/z_0 = 10^3$ and 10^5, while for $\lambda/z_0 = 10^7$, instabilities in the shooting method grow to corrupt the solution near the upper boundary. It is important, however, to note that the stress calculated by the shooting method is reasonable in the near-surface zone and that the calculation only begins to break down well above the surface.

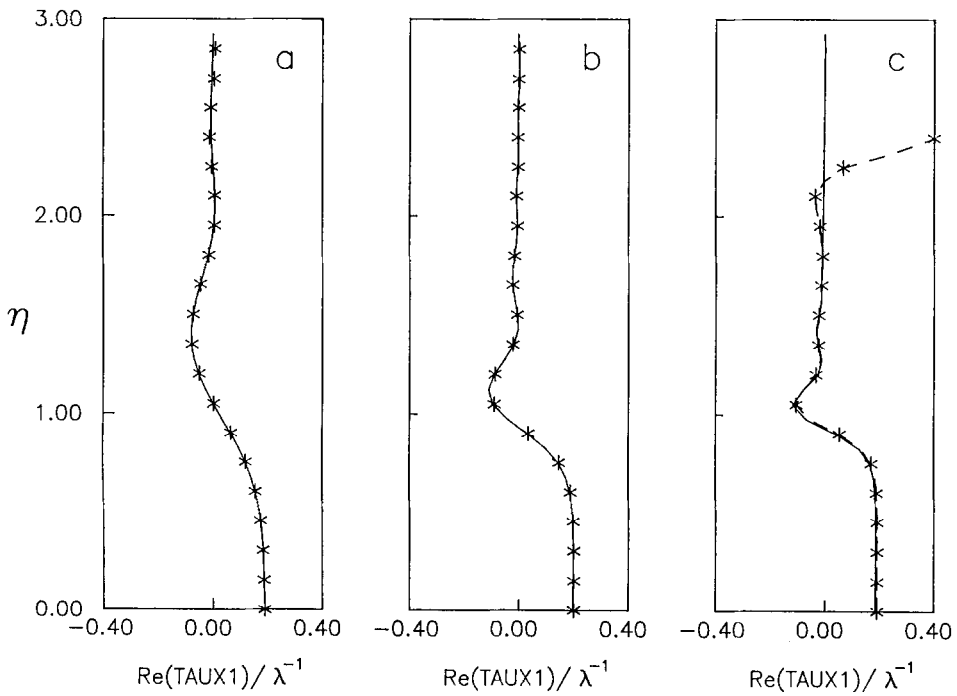

Fig. 4. Vertical profile of $\mathrm{Re}(\hat{\tau}_{x1})/\lambda^{-1}$ for a sinusoidal variation in topography for (a) $\lambda/z_0 = 10^3$, (b) $\lambda/z_0 = 10^5$, and (c) $\lambda/z_0 = 10^7$. Calculations made with 41 vertical levels. (Karpik – solid line; Beljaars *et al.* – asterisks.)

5. Concluding Remarks

It has been clearly demonstrated that the finite-difference method outlined here is significantly more robust than the shooting method for the solution of the MSFD model equations. However, one might argue that the difficulties with the shooting method occur only for extreme values of λ/z_0 (say, greater than 10^7) and at a height well above the surface. Thus, one might question the need for adopting the block tridiagonal finite-difference formulation.

It was mentioned earlier that for the mixing-length variant of the MSFD model, the shooting method apperared to work well. Extension of the model to incorporate the $E - \varepsilon$ and algebraic stress turbulence models caused the shooting method to become unstable for certain values of λ/z_0. The shooting method became ill-conditioned because of the addition of two second-order differential equations to the model set. If one wishes to extend the model further by adding additional closure equations or the thermodynamic equation, the model equation set will grow again. In this case, the shooting method will likely be inapplicable for an even wider range of λ/z_0 values. The present solution algorithm is considerably more robust and will, therefore, better accomodate modifications and/or additional equations as the MSFD model is developed to simulate increasingly complex problems.

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