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**Numerical methods for the linear vorticity equation
and for the advection-diffusion equation (**)**

A Bianca Manfredi con amicizia e stima

1 - Statement of the problem

Let Ω be a bounded open set of \mathbf{R}^2 with boundary Γ (piecewise C^1); we define for $T > 0$

$$Q_T = \Omega \times]0, T[\quad \Sigma_T = \Gamma \times]0, T[$$

and consider the following problem: *given the functions $z_0: \Omega \rightarrow \mathbf{R}$ ($z_0 \in L^2(\Omega)$), and $f: Q_T \rightarrow \mathbf{R}$, ($f \in L^2(Q_T)$), find a function $z: (x, t) \in Q_T \rightarrow z(x, t) \in \mathbf{R}$ solution of the equations*

$$(1.1) \quad \begin{aligned} \partial_t z + \operatorname{div}(\mathbf{b}Gz) + az - a_1 \Delta z &= f && \text{in } Q_T \\ \beta z = 0 & \quad \text{on } \Sigma_T && \quad z = z_0 && \text{in } \Omega \text{ for } t = 0 \end{aligned}$$

where $a, a_1 \in \mathbf{R}^+$, $\mathbf{b} = (b_1, b_2)^T$ is a given vector field, $\mathbf{b} \in L^\infty(\Omega) \times L^\infty(\Omega)$ such that

$$\int_{\Omega} \mathbf{b} \cdot \nabla \varphi \, d\Omega = 0 \quad \forall \varphi \in C_0^\infty(\Omega).$$

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$\beta z = z$ on Σ_T^1 and $\beta z = \frac{\partial z}{\partial n}$ on Σ_T^2 with $\Sigma_T^1 \cup \Sigma_T^2 = \Sigma_T$ (n denotes the unit outer normal vector to Γ),

$$(1.2) \quad G = I \quad \text{or} \quad G = L^{-1}$$

related to the advection-diffusion and to the linear barotropic vorticity equation respectively ([2], [12], [16]). L^{-1} is the inverse of the operator $L = -\Delta$ with domain $D(L) = \{\psi \in H^1(\Omega) \mid \psi = \psi_0 \text{ on } \Gamma\}$.

Let V be the completion in the Sobolev space $H^1(\Omega)$ of all smooth functions satisfying the boundary condition $\beta v = 0$ ($H_0^1(\Omega) \subset V \subset H^1(\Omega)$). The semidiscrete analogue of (1.1) will be based on the following *weak formulation*:

find a function $z: t \in [0, T] \mapsto z(t)$ such that

$$(1.3) \quad \begin{aligned} z &\in L^2(0, T; V) \cap C^0(0, T; L^2(\Omega)) & z(0) &= z_0 \\ \frac{d}{dt}(z(t), v) + (\operatorname{div}(\mathbf{b}Gz), v) + a(z, v) + a_1(\nabla z, \nabla v) &= (f, v) & \forall v \in V \end{aligned}$$

where $(,)$ stands for the usual scalar product in $L^2(\Omega)$ and $\frac{d}{dt}$ is taken in the sense of distributions on $]0, T[$. Now let V_h be a subspace of V , which consists of continuous piecewise bilinear functions in a quasiuniform rectangular mesh Ω_i ($\Omega = \cup \Omega_i$, $\Omega_i \cap \Omega_j = \emptyset$), (1.3) becomes:

find $z_h: t \in [0, T] \rightarrow z_h(t)$ such that

$$(1.4) \quad \begin{aligned} \frac{d}{dt}(z_h(t), v_h) + (\operatorname{div}(\mathbf{b}Gz_h), v_h) + a(z_h, v_h) + a_1(\nabla z_h, \nabla v_h) &= (f, v_h) & \forall v_h \in V_h \\ z_h(0) &= z_{0h}. \end{aligned}$$

In particular, if $\Omega = (0, l_x) \times (0, l_y)$, by introducing an uniform grid with steps $h_x = \frac{l_x}{n_x}$ and $h_y = \frac{l_y}{n_y}$, finite approximation spaces V^h can be constructed by means of bilinear splines functions $\varphi_i(x, y)$, $i = 1, \dots, n(n_x, n_y)$ so that $V^h = \operatorname{span}(\varphi_1, \varphi_2, \dots, \varphi_n)$.

By means of suitable quadrature formulas from (1.4) we have the o.d.e. system

$$(1.5) \quad \frac{du}{dt} + (A + BC)u = f$$

where A, B, C are $n \times n$ real matrices, where n is the dimension of V_h ,

$$(1.6) \quad \begin{aligned} A &= aI + a_1 A_1, & A_1 &= A_1^T \geq 0 \quad (\text{i.e. } x^T A_1 x \geq 0 \quad \forall x \in \mathbf{R}^n), & B &= -B^T \\ B\mathbf{e} &= 0 & \text{with } \mathbf{e} &= (1, 1, \dots, 1)^T, & C &= I \quad \text{or } C = A_1^{-1}. \end{aligned}$$

However, the results obtained in the following are valid for more general choices of C than (1.6); in the following we will assume that

$$(1.7) \quad C = C^T > 0 \quad CA_1 = A_1 C.$$

Equation (1.5) may be reduced to an equation with $C = I$; in fact let $C = LL^T$, $\tilde{\mathbf{u}} = L^T \mathbf{u}$, $\tilde{\mathbf{f}} = L^T \mathbf{f}$ then equation (1.5) becomes

$$(1.5)' \quad \frac{d\tilde{\mathbf{u}}}{dt} + (\tilde{A} + \tilde{B})\tilde{\mathbf{u}} = \tilde{\mathbf{f}}$$

where $\tilde{A} = L^T A L^{-T} = L^{-1} A L$ and $\tilde{B} = L^T B L$ is a skew-symmetric matrix.

We note that the use of the Galerkin method, together with suitable quadrature formulas, preserves the basic properties of the differential operators in (1.1). In particular, when $A > 0$ from (1.6) and (1.7) it follows that the real part of the eigenvalues of $A + BC$ is positive; thus, when the forcing term \mathbf{f} is time independent, a unique steady state solution exists and it is asymptotically stable (in the sense of Lyapunov). However, in solving the advection-diffusion equation, in the presence of a boundary layer, the cell Peclet number Pe must be chosen so that

$$(1.8) \quad Pe = \max\left(\frac{b_i h}{2a_1}\right) < 1$$

in order to avoid spurious oscillations. If condition (1.8) is satisfied and $A > 0$, it follows that the entries of $(A + B)^{-1}$ are positive. Thus, when the source is non-negative, the steady state solution is positive and spurious oscillations or *wiggles* do not occur. Note that the classical upwind schemes and streamline upwind methods lead to matrices for which some basic properties of matrices A and B are not satisfied, and consequently the maximum principle property is not necessarily preserved [6]. More recent Petrov-Galerkin formulations overcome most of the limitations found in Galerkin and upwind methods [1], [3], [7]. Reviews of the numerical methods for solving the advection-diffusion equation and of the development of the upwind techniques are presented in [1], [6], [10].

In the next Sections 2 and 3 we will consider time discretization schemes of equation (1.5) which lead to two-level and three-level difference equations respectively. In Section 4 we make some remarks on numerical calculations.

2 - Two-level difference equation

We integrate equation (1.5) by using the standard schemes ([8], [11], [15]). The algorithm is written in the following way

$$(2.1) \quad Mu_{j+1} = Nu_j + \Delta t f \quad j = 1, 2, \dots$$

where

$$(2.2) \quad M = I + \frac{1}{2}(1 - \alpha)\Delta t(A + BC) \quad N = I - \frac{1}{2}(1 + \alpha)\Delta t(A + BC)$$

and $-1 \leq \alpha \leq 1$; this choice assures that $\det M > 0$; here $M - N$ is a splitting of the matrix $\Delta t(A + BC)$. The following theorem can be proved.

Theorem 1. *Let M and N be given by (2.2) and let $g_0(\Delta t, \alpha)$ be the spectral radius $\rho(M^{-1}N)$ of the matrix $M^{-1}N$. Then*

- (i) $g_0(\Delta t, \alpha) < 1$ for an arbitrary Δt and $\alpha \leq 0$;
- (ii) $g_0(\Delta t, 1) < 1$ for $\Delta t \leq \min_i \left(\frac{2 \operatorname{Re}(\lambda_i)}{|\lambda_i|^2} \right)$

where λ_i are the eigenvalues of $A + BC$.

Proof. (i) From (2.2) by direct calculation we obtain $M^{-1}N = C^{-\frac{1}{2}} Z C^{\frac{1}{2}}$, where

$$Z = [I + \frac{1}{2}(1 - \alpha)\Delta t D]^{-1} [I - \frac{1}{2}(1 + \alpha)\Delta t D] \quad D = C^{\frac{1}{2}}(A + BC)C^{-\frac{1}{2}}.$$

From (1.6) and (1.7) it follows that

$$C^{\frac{1}{2}} A C^{-\frac{1}{2}} = C^{-\frac{1}{2}} A C^{\frac{1}{2}} \quad C^{\frac{1}{2}} B C^{\frac{1}{2}} = -(C^{\frac{1}{2}} B C^{\frac{1}{2}})^T;$$

thus, $D > 0$. The eigenvalues $\nu(Z)$ of Z can be expressed in terms of the eigenvalues $\mu(D)$

$$\nu(Z) = \frac{1 - \frac{1}{2}(1 + \alpha)\Delta t \mu(D)}{1 + \frac{1}{2}(1 - \alpha)\Delta t \mu(D)}.$$

From $\alpha \leq 0$ it follows that $|\nu(Z)| < 1$; then we have the thesis.

- (ii) See [15], Theorem 8.5.

3 - Three-level difference equation

The scheme described here is essentially related to commonly used implicit methods for solving special (linear and nonlinear) parabolic equations ([2], [4], [5], [9], [11]). We integrate equation (1.5) using a leap frog scheme for the advection term and standard schemes like (2.1)-(2.2) for the frictional and dispersion terms. The algorithm is written in the following way

$$(3.1) \quad M\mathbf{u}_{j+1} = N\mathbf{u}_{j-1} - K\mathbf{u}_j + 2\Delta t\mathbf{f} \quad j = 1, 2, \dots$$

$$(3.2) \quad M = (1 + a\Delta t)I + (1 - \alpha)\Delta t a_1 A_1 \quad N = (1 - a\Delta t)I - (1 + \alpha)\Delta t a_1 A_1 \quad K = 2\Delta t BC$$

and $-1 \leq \alpha \leq 1$; this choice assures that $M > 0$; here $M - N$ is a splitting of the matrix $2\Delta t(aI + a_1 A_1)$. To start (3.1) we could use the previous scheme (2.1) in order to compute \mathbf{u}_1 , using a finer time step.

The scheme (3.1) can be reduced to the two-level iteration process

$$(3.3) \quad \mathbf{u}_{j+1} = \mathcal{L}(\Delta t, \alpha)\mathbf{u}_j + \mathbf{f}$$

where

$$(3.4) \quad \begin{aligned} \mathbf{u}_j &= (\mathbf{u}_{j-1}, \mathbf{u}_j)^T & \mathbf{f} &= 2\Delta t(\mathbf{f}, \mathbf{f})^T \\ \mathcal{L}(\Delta t, \alpha) &= \begin{pmatrix} M & 0 \\ K & M \end{pmatrix}^{-1} \begin{pmatrix} N & -K \\ 0 & N \end{pmatrix}. \end{aligned}$$

The basic properties of the spectrum of $\mathcal{L}(\Delta t, \alpha)$ when $M > 0$ are shown in the following theorems.

Lemma 1. *Let $M - N = (M - N)^T > 0$, $M = M^T > 0$ and $CK = -(CK)^T$. Let the matrix \mathcal{L} be defined by (3.4) and λ be its eigenvalues. Then*

- (a) *the real eigenvalues λ are less than 1*
- (b) *the moduli of the complex eigenvalues λ are less than 1.*

Proof. The eigenvalue equation for the matrix (3.4) is given by

$$(3.5) \quad \mathcal{L} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}.$$

If λ is also an eigenvalue of $M^{-1}N$ we have $(M - N)\mathbf{u} = (1 - \lambda)M\mathbf{u}$, and it follows that λ is real and less than 1. If λ is not an eigenvalue of $M^{-1}N$, then from

(3.5) we obtain

$$(3.6) \quad \mathbf{u} = T^2(\lambda)\mathbf{u} \quad \text{with} \quad T(\lambda) = \sqrt{\lambda}(\lambda M - N)^{-1}K.$$

(3.6) is equivalent to the two equations

$$(3.7) \quad \left(\sqrt{\lambda}M - \frac{1}{\sqrt{\lambda}}N\right)\mathbf{w} = \mp K\mathbf{w}.$$

Let $\lambda = re^{i\sigma}$; we have $\sqrt{\lambda} = re^{i(\frac{\sigma}{2} + j\pi)}$, $j = 0, 1$. The real and imaginary parts of (3.7) are

$$(3.8) \quad Q_R \mathbf{w}_R - Q_I \mathbf{w}_I = \mp K \mathbf{w}_R \quad Q_I \mathbf{w}_R + Q_R \mathbf{w}_I = \mp K \mathbf{w}_I$$

where \mathbf{w}_R and \mathbf{w}_I are the real and imaginary parts of the vector \mathbf{w} and

$$(3.9) \quad Q_R = r^{-\frac{1}{2}} \cos\left(\frac{\sigma}{2} + j\pi\right)(rM - N) \quad Q_I = r^{-\frac{1}{2}} \sin\left(\frac{\sigma}{2} + j\pi\right)(rM + N).$$

Since CK is skew-symmetric, from (3.8) we obtain

$$(3.10) \quad (\mathbf{w}_R^T C Q_R \mathbf{w}_R) + (\mathbf{w}_I^T C Q_R \mathbf{w}_I) = 0.$$

The matrix Q_R in (3.9) may be written in the form

$$(3.11) \quad Q_R = r^{-\frac{1}{2}} \cos\left(\frac{\sigma}{2} + j\pi\right)[(r-1)M + (M-N)].$$

If $r \geq 1$ then

$$(3.12) \quad C[(r-1)M + (M-N)] > 0.$$

Therefore from (3.10)-(3.12) it follows that $\cos\left(\frac{\sigma}{2} + j\pi\right) = 0$, $j = 0, 1$; thus, $\sigma = \mp\pi$ and the eigenvalues $\lambda = re^{i\sigma} = r \cos(\mp\pi) = -r$ are real and negative; then (a) and (b) are true.

Theorem 2. Assume (1.6), (1.7), (3.2) and (3.4) with $\alpha \leq 0$. Let $g(\Delta t, \alpha) = \rho(\mathcal{L})$. Then, $g(\Delta t, \alpha) < 1$ if

- (i) $a_1 A_1 > 0 \quad \Delta t < \tau(A) \quad \alpha^* < \alpha \leq 0$
- (ii) $a_1 A_1 > 0 \quad \text{arbitrary } \Delta t \quad \alpha < \alpha^*$
- (iii) $a_1 A_1 \geq 0 \quad \Delta t < \|BC\|^{-1}$

where

$$(3.13) \quad \begin{aligned} \alpha^* &= -\sqrt{\mu^2(A) + \|BC\|^2} (a_1 \mu(A_1))^{-1} \\ \tau(\alpha) &= [\alpha a_1 \mu(A_1) + \sqrt{\mu^2(A) + \|BC\|^2}]^{-1} \\ \mu(A) &= \text{minimum eigenvalue of the matrix } A. \end{aligned}$$

Proof. Because of Lemma 1 we consider only the case of real and negative eigenvalues of \mathcal{L} .

(i) Let $\lambda = -r$, $r > 0$; (3.7) gives

$$(3.14) \quad (rM + N)z = \mp i \sqrt{r} Kz.$$

Suppose $r \geq 1$, then we have $rM + N = (r-1)M + (M-N) > 0$. Thus, from (3.14) it follows

$$(3.15) \quad 1 \leq \frac{r^{\frac{1}{2}} \|K\|}{\mu(rM + N)} = r^{\frac{1}{2}} \frac{2 \Delta t \|BC\|}{rp + q}$$

and then

$$(3.16) \quad r^2 p^2 + 2r[pq - 2\Delta t^2 \|BC\|^2] + q^2 \leq 0$$

where

$$p = 1 + \Delta t(a + (1 - \alpha)a_1 \mu(A_1)) \quad q = 1 - \Delta t(a + (1 + \alpha)a_1 \mu(A_1)).$$

From (3.16), if $\Delta t^2 \|BC\|^2 - pq \leq 0$, that is when

$$(3.17) \quad (\alpha^{*2} - \alpha^2)(a_1 \mu(A_1))^2 \Delta t^2 + 2\alpha a_1 \mu(A_1) \Delta t - 1 \leq 0$$

then $\lambda = -r$ is not an eigenvalue of $\mathcal{L}(\Delta t, \alpha)$. The inequality (3.17) is satisfied when $\alpha^* < \alpha \leq 0$ and $0 < \Delta t < \tau(\alpha)$. Hence the thesis.

The statements (ii) and (iii) follow by inspection from (3.17).

4 - Relaxation process

Now we show that the matrix (3.4) may be reduced to a relaxation matrix for a special choice of $\alpha = \alpha(\Delta t)$. Let us assume $a > 0$ and let

$$(3.18) \quad \omega = 2a \Delta t (1 + a \Delta t)^{-1} \quad \alpha = -(a \Delta t)^{-1} - \frac{2}{\omega}.$$

From (3.2) and (3.18) it follows that

$$(3.19) \quad M = 2 \Delta t \omega^{-1} A_1 \quad N = 2 \Delta t (1 - \omega) \omega^{-1} A.$$

Thus, the matrix (3.4) is the two block successive relaxation matrix associated to the 2-cyclic matrix

$$(3.20) \quad \begin{pmatrix} M - N & 0 \\ K & M - N \end{pmatrix} = 2 \Delta t \begin{pmatrix} A & BC \\ BC & A \end{pmatrix}$$

and equation (3.1) becomes

$$(3.21) \quad \omega^{-1} A \mathbf{u}_{j+1} = (1 - \omega) \omega^{-1} A \mathbf{u}_j - BC \mathbf{u}_j + \mathbf{f}.$$

It is easy to prove the following [15].

Theorem 3. *Assume (3.18) and (3.19) with $a > 0$ and*

$$c = \sqrt{1 + \rho^2 (A^{-1} BC)}.$$

Then we have $\min_{\Delta t} g(\Delta t, -(a \Delta t)^{-1}) = (c - 1)(c + 1)^{-1}$

and the minimum is obtained for $\Delta t = (ac)^{-1}$. Thus (3.3) is an underrelaxation process with optimum underrelaxation factor $\omega = 2(1 + c)^{-1}$.

At last we note that equation (3.21) can be regarded as a generalized conjugate gradient process [17] when ω is chosen in the following way

$$\omega_{j+1} = \left(1 + \frac{r_j}{r_{j-1} \omega_j}\right)^{-1} \quad j = 1, 2, \dots$$

where $r_j = \mathbf{v}_j^T A \mathbf{v}_j$ $\mathbf{v}_j = A^{-1} (\mathbf{f} - (A + BC) \mathbf{u}_j)$ $\omega_1 = 1$.

5 - Remarks on numerical calculations

As sample problems, we studied the wind-driven circulation (related to the classical Stommel problem [13]) and dispersion processes in the ocean and in (semi-)enclosed seas using depth-averaged models in two space dimensions.

Circulation problems

In equation (1.1), with $G = L^{-1}$, $b_2 = 0$, $\beta z = z$, z is the *vorticity*. The *veloci-*

ty field is determined by the *stream function* ψ given by $\Delta\psi = z$ in Ω and $\psi = 0$ on Γ . The region Ω is the unit square, the data are $b_1 = 1$, $\alpha = 0.05$, $a_1 = 0.00005$ and the *driving force* f , the curl of the wind stress, is given by

$$f = \pi \sin(\pi y) \quad \text{or} \quad f = 2\pi \sin(2\pi y)$$

corresponding to a single-gyre or a double-gyre field respectively. The number of grid points is of order 50×50 or 100×100 .

The two-level scheme (2.1)-(2.2) have been applied to equation (1.5)', in which \tilde{A} and \tilde{B} are band-matrices as A and B . The system (2.1) may be solved either by an LU decomposition of the matrix $M = I + \frac{1}{2}(1 - \alpha)\Delta t(\tilde{A} + \tilde{B})$ or by means of a generalized conjugate gradient method [17].

The three-level scheme (3.1)-(3.2) can be easily applied to equation (1.5). The system (3.1) may be solved either by an LL^T decomposition of the matrix $M = (1 + a\Delta t)I + (1 - \alpha)\Delta t a_1 A_1$ or by means of fast Helmholtz operator solver [14].

The *spectral radius* $g(\Delta t, \alpha)$ of $\mathcal{L}(\Delta t, \alpha)$, defined in (3.4), has been computed for different values of h , Δt and α in the range $-c \leq \alpha \leq 0$, where c is defined as in Theorem 3. $g(\Delta t, \alpha)$ and the bound $\tau(\alpha)$ for Δt defined in (3.13) are weakly dependent on h . The trend of $g(\Delta t, \alpha)$ versus Δt is similar to that of the spectral radius versus the relaxation parameter for the relaxation processes. $g(\Delta t, \alpha)$ has a minimum for a $\Delta t = \tau_m(\alpha)$ decreasing with α . The upper bound $\tau(\alpha)$ for Δt is lightly less than $\tau_m(\alpha)$. Numerical computations of the steady state solution, starting from the state of rest, have been performed. Let $J(\Delta t, \alpha)$ be the number of time iterations necessary to reach the steady state, assuming a suitable stopping criterion; values of Δt smaller than $\tau_m(\alpha)$ must be used to have convergence of $J(\Delta t, \alpha)\Delta t$.

Dispersion problems

Numerical simulations of dispersion processes of a passive pollutant released in a closed sea have been performed by using the steady velocity fields computed as described above and suitably normalized. In equation (1.1), with $G = I$, $\beta z = \frac{\partial z}{\partial n}$, z is the *concentration of the pollutant dissolved in water*. These boundary conditions imply the conservation of the total mass of the pollutant and the corresponding steady state problem is singular. However, it is possible to show the stability of the iteration processes which converges to the meaningful steady state.

Given the numerical viscosity a_1 ($10^2 \text{ m}^2 \text{ s}^{-1}$, $10^4 \text{ m}^2 \text{ s}^{-1}$) and of the maximum velocity $\sqrt{b_1^2 + b_2^2}$ (1 ms^{-1}) in the basins considered (surface = 10^{10} m^2 , 10^{12} m^2), the maximum size of the grid mesh h (10^3 m , 10^4 m) is determined by the inequality (1.8) $Pe < 1$; it follows that the number of grid points is 50×50 , 100×100 .

In this case, the two-level (2.1)-(2.2) and three-level (3.1)-(3.2) schemes can be directly applied to equation (1.5); the systems (2.1) and (3.1) can be solved as described above. By assuming $\alpha = 0$, the two schemes have the same order of approximation equal to 2 and produce very similar results.

Steady state circulation problem

We have stated in Section 4 that the block successive under-relaxation process (3.21) may be regarded as a Widlund algorithm [17]. We considered the following elliptic boundary value problem (a special time independent problem of (1.1) with $z = \Delta\psi$, $a_1 = 0$, $b_2 = 0$, $\beta z = z$ also used in [17])

$$\Delta\psi + b_0 \frac{\partial\psi}{\partial x} = c \sin(\pi y L^{-1})$$

in the square of side $l = 10^6 \text{ m}$ and $\psi = 0$ on the boundary; the parameter $b_0 = b_1 a^{-1}$, in the range 10^{-5} m^{-1} , 10^{-4} m^{-1} , is the ratio between the gradient of the planetary vorticity and the size of the bottom friction [13] and $c = \frac{\pi}{2} 10^{-6} \text{ s}^{-1}$. Calculations were performed for different values of b_0 to compare the two methods. For a case with 50×50 grid points, we found that the number of iterations required is approximately $15 \times 10^5 b_0$ for the process (3.21), while it is $3 \times 10^5 b_0^{0.7}$ for the Widlund process.

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Sommario

Si propone un metodo semidiscreto di Galerkin per l'equazione lineare della vorticità e per l'equazione avvezione-diffusione.

Si effettua una analisi della stabilità per schemi numerici iterativi a due e tre livelli.

Alcuni risultati numerici sono confrontati e discussi.
