Journal of Computational Physics **172,** 917–923 (2001)
doi:10.1006/jcph.2001.6857, available online at http://www.idealibrary.com on IDEAL®

NOTE

A Note on the Regularization of the Discrete Poisson–Neumann Problem

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Received February 2, 2001; revised May 30, 2001

Key Words: Poisson equation; Neumann boundary conditions; compatibility condition; solvability condition; incompressible flow; pressure Poisson equation; projection methods; pressure-correction methods.

The time integration of the equations of incompressible flow using (a) the velocity–pressure formulation in conjunction with the consistent or simplified pressure Poisson equation, (b) a projection method, or (c) a pressure–correction method, requires solving a Poisson equation for the pressure or for an auxiliary projection function used to approximate the pressure subject to the Neumann boundary condition over the solid boundaries of the flow. In the case of the pressure Poisson equation, an inhomogeneous Neumann boundary condition arises by projecting the Navier–Stokes equation normal to the boundaries, and then using the specified boundary conditions for the velocity to simplify the viscous and inertial contributions [1]. In the case of projection or pressure–correction methods, homogeneous or inhomogeneous Neumann boundary conditions for the projection function arise according to the selected boundary conditions for the intermediate velocity computed by integrating in time the Navier–Stokes equation in the absence of, or using extrapolated values for, the pressure gradient [2].

Now, it is well known that when the Neumann boundary condition is required over all external boundaries of an internal solution domain, the Poisson equation

$$\nabla^2 f = g \tag{1}$$

has a solution for the requisite function f only when the compatibility condition, requiring that the integral of the source function g over the domain of solution be equal to the net flow

rate expressed by the boundary integral of the normal derivative of f, is satisfied. In the case of a two-dimensional solution domain in the xy plane, denoted by D, the compatibility condition requires

$$\int_D g(x, y)\, dx\, dy = \int_C q\, dl, \tag{2}$$

where C is the boundary of D, $q \equiv \partial f/\partial n = \mathbf{n} \cdot \nabla f$ is the specified normal derivative, $\mathbf{n}$ is the unit vector normal to C pointing outward, and dl is the differential arc length along C. When the compatibility condition (2) is fulfilled, the Poisson equation (1) has a solution that can be determined up to an arbitrary constant. When the compatibility condition is not fulfilled, a solution cannot be found.

The spatial discretization of (1) by finite-difference, finite-volume, and some implementations of the finite-element method, replaces the Poisson equation with a linear algebraic system for the vector $\mathbf{w}$,

$$\mathbf{A} \cdot \mathbf{w} = \mathbf{b}, \tag{3}$$

where the right-hand side $\mathbf{b}$ incorporates the source term g and the specified Neumann boundary conditions. If the numerical discretization is consistent, the matrix $\mathbf{A}$ is singular: a vector $\mathbf{u}$ with equal elements is an eigenvector of $\mathbf{A}$ corresponding to the null eigenvalue, $\mathbf{A} \cdot \mathbf{u} = \mathbf{0}$. For system (3) to have a solution, the right-hand side must be orthogonal to the eigenvector of the transpose of $\mathbf{A}$ corresponding to the null eigenvalue, denoted by $\mathbf{v}$ and satisfying $\mathbf{v}^T \cdot \mathbf{A} = \mathbf{0}$, yielding the solvability condition

$$\mathbf{v}^T \cdot \mathbf{b} = \mathbf{0}. \tag{4}$$

Since the matrix $\mathbf{A}$ is generally nonsymmetric, the eigenvectors $\mathbf{u}$ and $\mathbf{v}$ are not necessarily identical.[1]

The solvability condition (4) is, in fact, the discrete implementation of the compatibility condition (2). In this light, the left-hand side of (4) is recognized as the implementation of a numerical integration quadrature pertinent to the areal and line integrals on the left- and right-hand side of (2). The particular nature of this quadrature depends on the structure of the matrix $\mathbf{A}$ which is determined by the method selected to discretize the Laplacian on the right-hand side of (1). This observation reveals an intimate relation between a numerical differention matrix and the singular eigenvector of its transpose with reference to numerical integration.

In practice, because of discretization error, the solvability condition is not always fulfilled, and the linear system (3) does not always have a solution. In the majority of fluid dynamics applications, this essential difficulty is overlooked, and a solution is found by iteration using, for example, the Jacobi, the Gauss–Siedel, or the SOR method. The iterations amount to stepping in time on the borderline of numerical stability based on the unsteady diffusion–reaction equation that emerges by adding the time derivative $\partial f/\partial t$ to the right-hand side of (1). It is clear then that if the compatibility condition is not fulfilled, a convergent solution corresponding to the steady state cannot be found. In most implementations, only a few iterations are carried out, and a solution of unknown accuracy is obtained, as discussed by de Foy and Dawes [3].

[1] The Galerkin finite-element method and the finite-difference method implemented with biased inward differences give a symmetric coefficient matrix at the penalty of reduced accuracy.

The difficulty has been noted and addressed by two groups of authors. Abdallah, Sotiropoulos, and Tafti developed consistent finite-difference discretizations for Cartesian and curvilinear collocated (nonstaggered) grids that ensure the automatic satisfaction of the compatibility condition while producing nonoscillatory solutions that do not suffer from odd–even coupling [4–7]. de Foy and Dawes [3] recently developed a consistent discretization for finite-volume unstructured grids. Although these methods undoubtedly represent the optimal approach, the additional amount of necessary work, the possible introduction of numerical compressibility, and some loss of generality are practical disadvantages.

A second group of authors, dating back to Briley (1974) [8] opted to modify the source term of the Poisson equation, but not necessarily the boundary conditions, thereby replacing the linear system (3) with the modified system

$$\mathbf{A} \cdot \mathbf{w} = \mathbf{b} - \epsilon\, \mathbf{c}, \tag{5}$$

where $\mathbf{c}$ is a suitable vector normalized so that $\mathbf{c}^T \cdot \mathbf{c} = 1$, and the constant ϵ on the right-hand side is adjusted to ensure the satisfaction of the solvability condition [9–11]. When the adjoint eigenvector $\mathbf{v}$ is available, we may enforce the solvability condition to compute $\epsilon = (\mathbf{v}^T \cdot \mathbf{b})/(\mathbf{v}^T \cdot \mathbf{c})$. In practice, the eigenvector $\mathbf{v}$ may be either computed directly or compiled by inspection in terms of integration quadrature weights. A practical method of computing ϵ without reference to $\mathbf{v}$ is discussed by Pozrikidis [12]. When the linear system (3) is solved by iteration, the regularization embodied by (5) may be implemented simply by shifting all components of the solution vector $\mathbf{w}$ by the same amount after each iteration, so that one arbitrary component is anchored at a fixed value.

In this note, we argue that the optimal way of regularizing the linear system (3) is by projecting the right-hand side onto the orthogonal complement of the adjoint eigenvector $\mathbf{v}$, thereby obtaining the regularized system

$$\mathbf{A} \cdot \mathbf{w} = (\mathbf{I} - \mathbf{v}\mathbf{v}^T) \cdot \mathbf{b}, \tag{6}$$

where $\mathbf{v}^T \cdot \mathbf{v} = 1$. By construction then, the solvability condition is fulfilled. Comparing (5) and (6), we identify the otherwise arbitrary vector $\mathbf{c}$ with $\mathbf{v}$, and the constant ϵ with the projection $\mathbf{v}^T \cdot \mathbf{b}$. The regularization expressed by (6) amounts to uniformly perturbing the source term in the Poisson equation as well as the boundary conditions in a specific way.

To investigate the performance of the method based on (6), we consider the solution of Poisson's equation in a rectangular domain confined between $0 < x < a$ and $0 < y < b$, where the source term is given by

$$g(x, y) = -\frac{1}{a^2} e^{-(x+y)/\delta} + \frac{\delta^2}{a^3 b}\left(1 - e^{-a/\delta}\right)\left(1 - e^{-b/\delta}\right), \tag{7}$$

where δ is a specified length, and the homogeneous Neumann condition is required around the sides. The source term g was designed so that the function f is dimensionless, and the integral of g over the solution domain vanishes so that the compatibility condition is satisfied.

The solution domain was discretized into a uniform $N \times M$ Cartesian grid, and the Laplacian was approximated using the five-point centered difference formula. In one implementation, termed I1, phantom nodes are introduced to approximate the Neumann boundary condition using centered differences, and the Poisson equation is applied at both the interior and boundary nodes. In a second implementation, termed I2, the Neumann boundary

condition is implemented using second-order, one-sided differences biased toward the interior, and the Poisson equation is applied only at the interior nodes. In both cases, the difference equations expressing the Neumann boundary condition are combined with the finite-difference approximation of the Laplacian at the boundary or near-boundary nodes to produce a modified five-point formula and a suitable right-hand side. The matrix $\mathbf{A}$ is nonsymmetric in both implementations.

To simplify the nomenclature, we identify regularization done with uniform perturbation in the source term alone as R1, and regularization done with $\mathbf{c} = \mathbf{v}$ as R2. Computations showed that when $N = M = 16$, $\delta = a$, and $a = b$, the projection distance ϵ for cases I1-R1 and I1-R2 is, respectively, equal to -1.728×10^{-5} and -1.678×10^{-5}. The corresponding values for cases I2-R1 and I2-R2 are 7.00×10^{-5} and 6.83×10^{-5}. These results confirm that regularization R2 minimizes the projection distance ϵ, and may therefore be endowed with the qualifier "optimal." Figure 1(a) shows the solution obtained with method

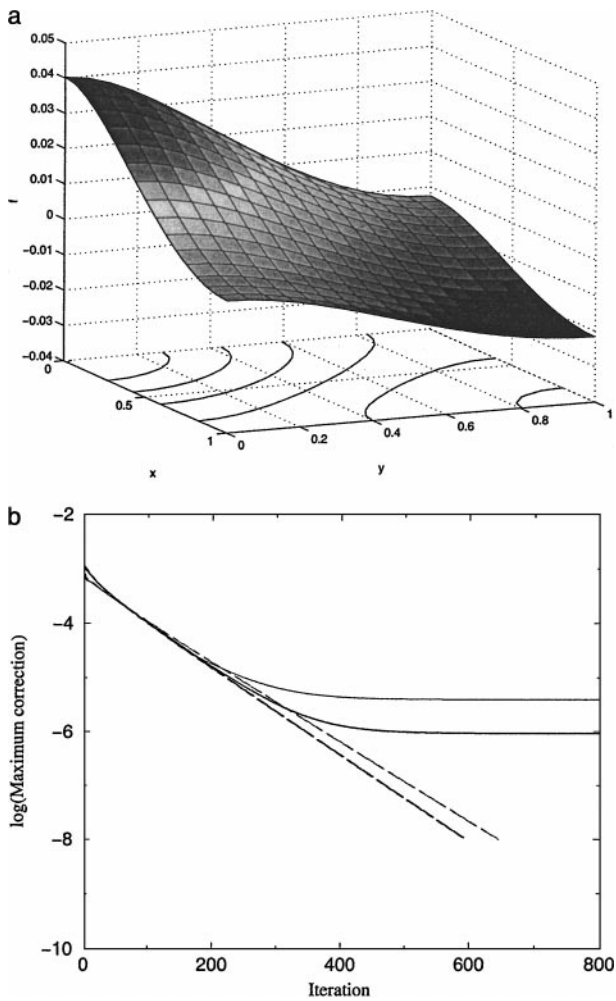

FIG. 1. (a) Solution of the Poisson–Neumann problem discussed in the text. (b) Effect of regularization on the convergence of the Gauss–Siedel iterations; the thick lines are for discretization I1, and the thin lines are for discretization I2; the solid, dashed, and long-dashed lines correspond, respectively, to no-regularization, R1, and R2; the dashed and long-dashed lines are virtually indistinguishable.

I1-R2 for $\delta = 0.5a$, and $a = b$. The corresponding solution obtained with R1 is virtually indistinguishable.

To illustrate the effect of regularization on the convergence of an iterative method for solving the Poisson equation, in Fig. 1(b) we plot the maximum correction in f against

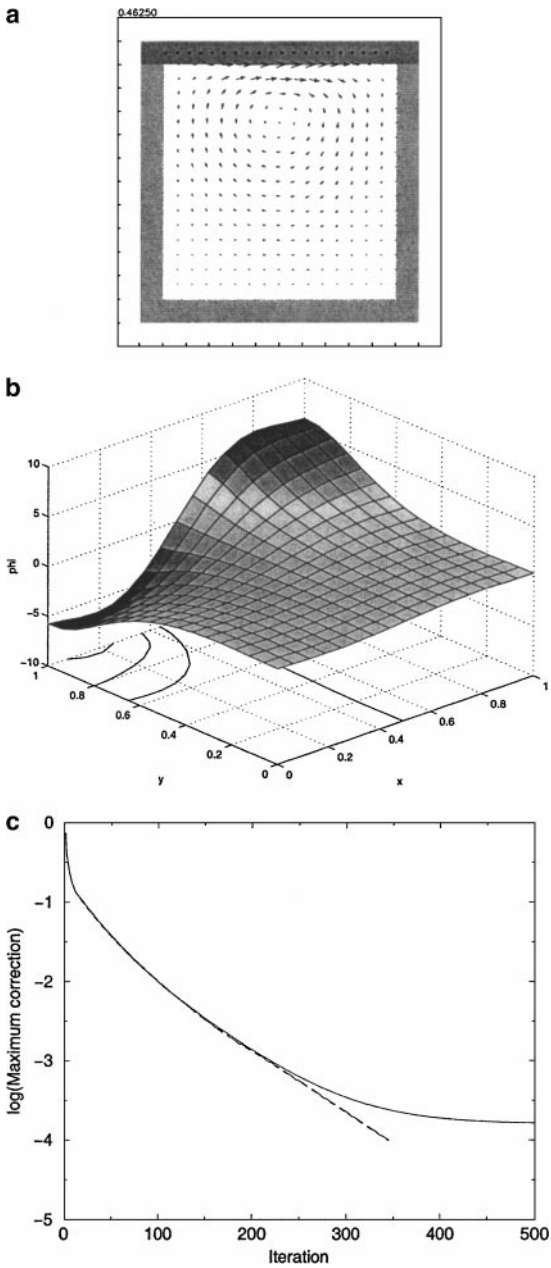

FIG. 2. (a) Instantaneous streamline pattern of flow in a square cavity driven by a translating lid with sinusoidal velocity distribution at Reynolds number $Re = 1.0$; (b) corresponding distribution of the projection function approximating the pressure. (c) Effect of regularization on the convergence of Gauss–Siedel iterations; the solid, dashed, and long-dashed lines correspond, respectively, to no-regularization, regularization R1, and regularization R2; the dashed and long-dashed lines are virtually indistinguishable.

the number of iterations on a linear-log scale corresponding to Fig. 1(a). The updates are done using the Gauss–Siedel method starting from the null initial state. Note that the iterations rely on the Neumann boundary conditions implemented in the finite-difference matrix for convergence. The thick lines in Fig. 1(b) correspond to discretization I1, and the thin lines correspond to discretization I2; the solid, dashed, and long-dashed lines correspond, respectively, to no-regularization, regularization R1, and regularization R2; note that the dashed and long-dashed lines are virtually indistinguishable. The results illustrate the divergence of the iterations in the absence of regularization, and reveal nearly identical performances for R1 and R2.

To further illustrate the performance of the method, we consider flow in a square cavity driven by a moving lid with a sinusoidal velocity distribution at Reynolds number $Re = UL/\nu = 1$, where U is the maximum lid velocity occurring at the mid-plane, L is the vcavity side length, and ν is the kinematic viscosity. The evolution of the flow is computed using a projection method on a nonstaggered grid, with the convection–diffusion steps treated implicitly by the Crank–Nicolson method. The projection function is computed by solving the Poisson equation with homogeneous Neumann boundary conditions over the cavity walls using implementation I1 [12]. The numerical method is discussed in detail in [13]. Figure 2(a) shows the instantaneous velocity vector field at dimensionless time $\hat{t} \equiv tU/L = 0.4825$, and Fig. 2(b) shows the corresponding distribution of the projection function which is nearly identical to the pressure. Regularization R1 requires $\epsilon = -0.00560$, and regularization R2 requires the lower value $\epsilon = -0.00544$, thus introducing a lesser amount of numerical compressibility, in agreement with the results of the model problem discussed earlier in this note. Figure 2(c) illustrates the performance of the iterative methods, showing the divergence of the Gauss–Siedel iterations in the absence of regularization.

In summary, regularization R2 was found to be optimal in the sense of minimal perturbation of the discrete Poisson–Neumann system, but its advantages should be weighed against the cost of computing the adjoint eigenvector of the null eigenvalue. The ease of implementation of regularization R1 with an iterative solver makes it a competitive alternative.

ACKNOWLEDGMENT

This research was supported by a grant provided by the National Science Foundation.

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