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A COMPARATIVE STUDY OF FINITE ELEMENT AND FINITE DIFFERENCE METHODS FOR CAUCHY-RIEMANN TYPE EQUATIONS

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ABSTRACT

A least squares formulation of the system $\operatorname{div}\underline{u} = \rho$, $\operatorname{curl}\underline{u} = \underline{\zeta}$ is surveyed from the viewpoint of both finite element and finite difference methods. Closely related arguments are shown to establish convergence estimates.

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Introduction

This paper concerns the three dimensional Cauchy-Riemann type equations

$$(1)\qquad \begin{aligned} \operatorname{div}\underline{u} = \rho,\ \operatorname{curl}\underline{u} = \underline{\zeta} \quad &\text{in } D \\ \underline{u}\cdot\underline{n} = 0 \quad &\text{on } \Gamma; \end{aligned}$$

D is a bounded domain in $\mathbb{R}^3$ with boundary Γ on which $\underline{n}$ is the outward normal. The functions $\rho, \underline{\zeta}$ are prescribed and satisfy the compatability conditons

$$(2)\qquad \int_D \rho \, d\pi = 0, \quad \operatorname{div}\underline{\zeta} = 0 \quad \text{in } D;$$

these express necessary conditons that the overdetermined first-order system (1) has a solution.

The numerical solution of these equations will be studied from both the finite element and finite difference points of view. Indeed, the major goal of this paper is to show how both approaches rest on very similar foundations. In so doing we hope our study may provide a point of contact between those familiar with the, largely separate, literature about each method.

In the case of the finite element method convergence estimates will be shown to result quite directly from proof techniques already common to the finite element literature. In contrast, many of these same techniques have played little or no role in the analysis of finite difference schemes and one of our principal objectives lies in clarifying their relevence to finite difference methods.

The Cauchy-Riemann type equations (1) were chosen for study because they are representative of a type of first-order systems that arise in problems from electromagnetics and fluid dynamics. For such systems, arbitrary finite differencce and finite element approximations to (1) are generally unsuitable. This is certainly true of all but a few finite element schemes based on Galerkin formulations [1], while simple finite difference approximations can present, among other difficulties, special problems in incorporating boundary conditions accurately.

In Part A notations used in this paper are introduced and the basic intergral identity

$$\text{(3)} \qquad \int_D [\,|\mathrm{curl}\,\underline{u}|^2 + |\mathrm{div}\,\underline{u}|^2] = \int_D |\mathrm{grad}\,\underline{u}|^2$$

is derived. This identity has found use in many applications (see, for example, [3] where it is used in a discussion of the Navier-Stokes equations). The derivation given in Section A.1 differs from (3) in appearence in order to highlight the structural properties of (1) when viewed as a first-order system.

The fact that (1) is well posed is an immediate consequence of (3) and the Lax-Milgram Theorem. This is described in Section A.2 both for completeness and because it shows the fundamental role the least squares ideas can play in discussing overdetermined systems like (1).

The derivation of a stable and optimally convergent finite element scheme is almost immediate from the material developed in Part A. The arguments, while standard, are included in Part B for completeness. It is interesting to note that, unlike other least squares approximations to first-order systems, these do not impose any restrictions on the finite element spaces [2].

In Part C an analogous development is given for the Keller box-scheme based, instead, on a least squares summation formulation. Here a summation by parts formula is used to obtain a summation identity analogous to (3) and results in a proof that the scheme is second order accurate. Of special interest is the fact that this development, also, is not restricted to uniform grids nor to grids obtained by images of uniform grids under a global mapping function. Thus, like the finite element schemes, it can also be used on irregular grids subject only to standard geometric constraints. Finally, we remark that the difference scheme employed here (c. f. [10] [12]) involves the variables on the same, rather than on staggered, grids in contrast to [5], [9].

Part A

A Least Squares Formulation

A1. An Integral Identity

In the following, $\underline{x} = (x_1,x_2,x_3)$ is a point in $\mathbb{R}^3$, $\partial_i \equiv \frac{\partial}{\partial x_i}$, and (ijk) indicates that the indices i,j,k are restricted to an even permutation of (123). Thus

$$\operatorname{div}\underline{u} = \sum_{i=1}^{3} \partial_i u_i ,$$

$$\operatorname{curl}\underline{u} = \left(\partial_j u_k - \partial_k u_j\right), \quad (ijk),$$

$$\operatorname{grad}\underline{u} = \left(\partial_i u_j\right).$$

With

$$(\underline{u},\underline{v}) \equiv [\mathrm{grad}\underline{u}:\mathrm{grad}\underline{v}] \equiv \sum_{i=1}^{3} \mathrm{grad}u_i \mathrm{grad}v_i,$$

we define

$$\|\underline{u}\|^2 \equiv \int_D (\underline{u},\underline{u})d\pi,$$

$$\|\underline{u}\|_0^2 \equiv \int_D |\underline{u}|^2 d\pi$$

and

$$\|\underline{u}\|_1^2 = \|\underline{u}\|^2 + \|\underline{u}\|_0^2.$$

The system (1) may be written in matrix form as

(A.1.1) $$L\underline{u} \equiv \sum_{i=1}^{3} A_i \partial_i \underline{u} = \underline{f}$$

where $\underline{f} = (\rho,\underline{\zeta})^T$ and

$$A_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Set

(A.1.2) $$B_i = A_k^T A_j, \quad (ijk).$$

It is easy to verify that

(A.1.3) $$\left.\begin{aligned} A_i^T A_i &= I, \\ B_i^T &= -B_i \end{aligned}\right\} \quad i = 1,2,3,$$

where I is the 3×3 identity matrix.

Recalling the definition $(\underline{u},\underline{v}) \equiv [\mathrm{grad}\underline{u}:\mathrm{grad}\underline{v}]$, integration by parts leads to the identity

(A.1.4) $$(L\underline{u})^T L\underline{v} = (\underline{u},\underline{v}) + \mathrm{div}\underline{q} - \Omega(\underline{u})\underline{v}$$

where, if $\underline{q} = (q_1,q_2,q_3)$,

(A.1.5) $$q_i \equiv \left(B_k^T\partial_j\underline{u}+B_j\partial_k\underline{u}\right)^T\cdot\underline{v}, \quad (ijk),$$

and $\Omega(\underline{u})$ is a vector with components Ω_i given by

(A.1.6) $$\Omega_i(\underline{u}) = \left(B_k^T\partial_j\partial_i\underline{u}^T+B_k\partial_i\partial_j\underline{u}^T\right), \quad (ijk).$$

Suppose $\underline{u}$ is smooth; since $B_k^T = -B_k$, then $\Omega(\underline{u}) = 0$. Also, in terms of the components of $\underline{u}$ and $\underline{v}$ the component q_i of $\underline{q}$ is easily verified to have the form

$$q_i = v_i\left(\partial_j u_j+\partial_k u_k\right) - \left(v_j\partial_j+v_k\partial_k\right)u_i, \quad (ijk)$$

Let

(A.1.7) $$\hat{q}_i = v_i\left(\partial_j u_j+\partial_k u_k\right) + u_i\left(\partial_j v_j+\partial_k v_k\right)$$

so that

$$q_i = \hat{q}_i - \left(\partial_j\left(v_j u_i\right)+\partial_k\left(v_k u_i\right)\right).$$

Since the expression in brackets is a surface divergence then

$$\int_\Gamma \underline{q}\cdot\underline{n}d\sigma = \int_\Gamma \hat{\underline{q}}\cdot\underline{n}d\sigma.$$

Integrating (A.1.4) and employing Gauss′ theorem

$$\int_D (L\underline{u})^T L\underline{v}\, d\pi = \int_D (\underline{u},\underline{v})\, d\pi + \int_\Gamma \hat{\underline{q}}\cdot\underline{n}\, d\sigma$$

Suppose $\underline{u}\cdot\underline{n} = \underline{v}\cdot\underline{n} = 0$ on Γ; the preceding remark implies that $\hat{\underline{q}}\cdot\underline{n} = 0$ on Γ so that

(A.1.9) $$\int_D (L\underline{u})^T L\underline{v}\, d\pi = \int_D (\underline{u},\underline{v})\, d\pi.$$

A2. Norm Estimates and Uniqueness

The goal here is to use tha basic identity (A.1.9) and the Lax-Milgram Theorem to show existence and uniqueness for the system

(A.2.1) $$L\underline{u} = \underline{f} \quad \text{in} \quad D, \qquad \underline{u}\cdot\underline{n} = 0 \quad \text{on} \quad \Gamma$$

where L is defined in (A.1.1). To do this we must first formulate (A.2.1) in terms of a bilinear form $a(\cdot,\cdot)$ on an apropriate space V. In particular we put

(A.2.2) $$a(\underline{v},\underline{w}) = \int_D L\underline{v}^T L\underline{w}\, d\pi = \int_D \{\mathrm{div}\underline{v}\cdot\mathrm{div}\underline{w} + \mathrm{curl}\underline{v}\cdot\mathrm{curl}\underline{w}\}\, d\pi$$

Moreover, we let

(A.2.3) $$V = \{\underline{v}\varepsilon\vec{L}^2(D): \underline{v}\cdot\underline{n} = 0 \text{ on } \Gamma,\ \mathrm{grad}\underline{v}\ \varepsilon\ \vec{L}^2(D)\}$$

with

(A.2.4) $$\|\underline{v}\| = \{\int_D (\underline{v},\underline{v})\, d\pi\}^{1/2} = \{\int_D [\mathrm{grad}\underline{v} : \mathrm{grad}\underline{v}]\, d\pi\}^{1/2}$$

This is a Hilbert space with the associated inner product

$$(A.2.5)\qquad \langle \underline{u},\underline{v}\rangle = \int_D (\underline{u},\underline{v})d\pi = \int_D (\mathrm{grad}\underline{u}:\mathrm{grad}\underline{v})d\pi.$$

That the bilinear form $a(\cdot,\cdot)$ satisfies the conditons of the Lax-Milgram Theorem [13] follows immediately from the integral identity (A.1.9), which can be written

$$(A.2.6)\qquad a(\underline{u},\underline{v}) = \int_D (\underline{u},\underline{v})d\pi.$$

Indeed, putting $\underline{v} = \underline{u}$ we obtain

$$(A.2.7)\qquad a(\underline{u},\underline{u}) = \|\underline{u}\|^2,$$

while

$$(A.2.8)\qquad |a(\underline{u},\underline{v})| \leq \|\underline{u}\|\|\underline{v}\|$$

is also clear.

It follows that given any bounded linear functional $G(\cdot)$ on V there is a unique $\underline{u}\varepsilon V$ for which

$$(A.2.9)\qquad a(\underline{u},\underline{v}) = G(\underline{v}) \quad \text{all } \underline{v}\varepsilon V;$$

moreover,

$$(A.2.10)\qquad \|\underline{u}\| \leq \|G\|.$$

Our final task is to choose $G(\cdot)$ so that (A.2.9) is equivalent to (A.2.1) - (A.2.2). Indeed, given $\rho\varepsilon L^2(D)$, $\underline{\zeta}\varepsilon\vec{L}^2(D)$ we put

$$(A.2.11)\qquad G(\underline{v}) = \int_D \underline{f}^T L u d\pi = \int_D \{\rho \mathrm{div}\underline{v} + \underline{\zeta}\cdot\mathrm{curl}\underline{v}\}d\pi.$$

Observe that

(A.2.12) $$|G(\underline{v})| \leq \|\underline{f}\|_0 \|L\underline{v}\|_0 = \|\underline{f}\|_0 \|\underline{v}\|$$

so that

(A.2.13) $$\|G\| \leq \|\underline{f}\|_0 = \{\|\rho\|_0^2 + \|\underline{\zeta}\|_0^2\}^{1/2}.$$

Moreover, (A.2.9) is equivalent to

(A.2.14) $$\int_D |L\underline{u}-\underline{f}|^2 d\pi = \int_D \{|\mathrm{div}\underline{u}-\rho|^2 + |\mathrm{curl}\underline{u}-\zeta|^2\} d\pi$$

be minmized over $\underline{v}\varepsilon V$. Thus, if the data $\rho,\underline{\zeta}$ satisfy the compatability conditons

(A.2.15) $$\int_D \rho d\pi = 0, \quad \mathrm{div}\underline{\zeta} = 0,$$

then the min in (A.2.14) will be zero and the minimizing function $\underline{u}\varepsilon V$ will satisfy (A.2.1).

In conclusion, it follows that if

(A.2.16) $$\rho\varepsilon L_0^2(D) \equiv \{\psi\varepsilon L^2(D)\colon \int_D \psi d\pi = 0\}$$

(A.2.17) $$\underline{\zeta}\varepsilon \vec{L}^2_{\mathrm{div}}(D) \equiv \{\underline{v}\varepsilon\vec{L}^2(D)\colon \mathrm{div}\underline{v} = 0\varepsilon D\}$$

are given then there is a unique $\underline{u}\varepsilon V$ such that (A.2.1) holds. Moreover,

(A.2.18) $$\|\underline{u}\| \leq (\|\rho\|_0^2 + \|\underline{\zeta}\|_0^2)^{1/2}.$$

Part B

A Finite Element Treatment

B1. Least Squares Formulation

Since the infinite dimensional problem (A.2.1) - (A.2.2) has a natural characterization (via the Lax-Milgram Theorem) in terms of a least squares formulation, it is reasonable to consider approximations based on these ideas. Indeed, Let

$$V_h \subseteq V \tag{B.1.1}$$

be a finite dimensional subspace parameterized by $h > o$. We seek a $\underline{u}_h \varepsilon V_h$ which minimizes

$$\int_D |L\underline{v}^h - \underline{f}|^2 = \int_D \left\{ |\mathrm{div}\underline{v}^h - \rho|^2 + |\mathrm{curl}\underline{v}^h - \underline{\zeta}|^2 \right\} d\pi \tag{B.1.2}$$

as $\underline{v}^h$ varies over V_h. Observe that if $a(\cdot,\cdot)$ and $G(\cdot)$ are defined as in Section A.2, then $\underline{u}_h$ is a minimizing function if and only if

$$a\left(\underline{u}_h, \underline{v}^h\right) = G\left(\underline{v}^h\right) \quad \text{all} \quad \underline{v}^h \varepsilon V_h. \tag{B.1.3}$$

Moreover, application of the Lax-Milgram Theorem to V_h shows $\underline{u}_h \varepsilon V_h$ is uniquely determined by (B.1.3). Once a basis is chosen for V_h, (B.1.3) reduces to a set of symmetric positive definite algebraic equations.

B2. Error Estimates

Combining (A.2.9) and (B.1.3) we see that

$$a(\underline{u}-\underline{u}^h,\underline{v}^h) = 0 \quad \text{all} \quad \underline{v}^h \varepsilon V_h. \tag{B.2.1}$$

This orthogonality condition is central to all error estimates. Indeed, first note that if $\tilde{\underline{u}} \varepsilon V_h$ is given, then (B.2.1) gives

$$a(\underline{u}-\tilde{\underline{u}}^h,\underline{u}-\tilde{\underline{u}}^h) = a(\underline{u}-\underline{u}_h,\underline{u}-\underline{u}_h) + a(\underline{u}_h-\tilde{\underline{u}}^h,\underline{u}_h-\tilde{\underline{u}}^h). \tag{B.2.2}$$

Thus

$$\|\underline{u}-\tilde{\underline{u}}^h\|^2 = \|\underline{u}-\underline{u}_h\|^2 + \|\underline{u}_h-\tilde{\underline{u}}^h\|^2.$$

It follows that $\underline{u}_h$ is a best approximation in the sense that

$$\|\underline{u}-\underline{u}_h\| = \inf \|\underline{u}-\tilde{\underline{u}}^h\| \leqslant \inf \|\underline{u}-\tilde{\underline{u}}^h\|_1, \tag{B.2.3}$$

where the inf is taken over all $\tilde{\underline{u}}^h$ in V_h.

In particular, if V_h consist of piecewise linear elements, then (B.2.3) gives

$$\|\underline{u}-\underline{u}_h\| \leqslant Ch\|\underline{u}\|_2, \tag{B.2.4}$$

where h is a generic mesh spacing. Here $\|\cdot\|_2$ is the Sobolev norm containing all derivatives up to second order.

To estabilsh L_2 estimates we use the standard "duality argument." The starting point is the following adjoint problem for $\underline{w}\varepsilon V$, where the error $\underline{u} - \underline{u}_h$ is the data:

(B.2.5) $$a(\underline{v},\underline{w}) = \int_D \underline{v}^T[\underline{u}-\underline{u}_h]d\pi \quad \text{all} \quad v\varepsilon V.$$

Suppose for the moment that (B.2.5) can be solved for $\underline{w}$, and

(B.2.6) $$\|\underline{w}\|_2 \leq C\|\underline{u}-\underline{u}_h\|_0.$$

In this case we put $\underline{v} = \underline{u}-\underline{u}_h$ in (B.2.5) to get

(B.2.7) $$a(\underline{u}-\underline{u}_h,\underline{w}) = \int_D |\underline{u}-\underline{u}_h|^2 = \|\underline{u}-\underline{u}_h\|_0^2 \ ;$$

using orthogonality (i.e. (B.2.1)) we get

(B.2.8) $$a(\underline{u}-\underline{u}_h,\underline{w}-\underline{w}^h) = \|\underline{u}-\underline{u}_h\|_0^2$$

for any $\underline{w}^h$ in V_h. Thus

(B.2.9) $$\|\underline{u}-\underline{u}_h\| \ \|\underline{w}-\underline{w}^h\| \geq \|\underline{u}-\underline{u}_h\|_0^2.$$

We select $\underline{w}_0^h \varepsilon V^h$ so that

(B.2.10) $$\|\underline{w}-\underline{w}^h\| \leq Ch\|\underline{w}\|_2.$$

Thus, with (B.2.6) we get

(B.2.11) $$\|\underline{u}-\underline{u}_h\|_0 \leq Ch\|\underline{u}-\underline{u}_h\|$$

Therefore, if linear elements are used

$$\|\underline{u}-\underline{u}_h\|_0 \leq Ch^2\|\underline{u}\|_2.$$

The final task is to check (B.2.5) for solvability as well as the a priori bound (B.2.6). Rewriting (B.2.5) we get

$$\text{(B.2.12)} \qquad \int_D L\underline{v}^T L\underline{w}\,d\pi = \int_D \underline{v}^T(\underline{u}-\underline{u}_h)\,d\pi \quad \text{all } \underline{v}\varepsilon V.$$

Suppose $\underline{v}\varepsilon V$ and $\underline{v}=0$ on Γ. Then integration by parts gives

$$\text{(B.2.13)} \qquad \int_D \underline{v}^T L^* L\underline{w}\,d\pi = \int_D \underline{v}^T(\underline{u}-\underline{u}_h)\,d\pi \quad \text{all } \underline{v}\varepsilon V,$$

where

$$L^*L = \text{curl curl-grad div} = \vec{\Delta}.$$

Thus defining $\underline{w}$ by

$$L^*L\underline{w} = \underline{u}-\underline{u}_h \quad \text{in } D$$

$$\underline{w} = 0 \qquad \text{on } \Gamma$$

it follows that $\underline{w}$ satisfies (B.2.5). Moreover, the a priori bound (B.2.6) follows from the theory of second order elliptic equations [8].

Part C

A Finite Difference Approach

C1. Notational Preliminaries;

Box Variables.

The notations about to be introduced are most naturally interpreted when D can be subdivided into cells $\{\pi\}$ each of which is a rectangular box. In a later section we shall indicate how more general subdivisions may be treated explicitly.

Following Keller [7] we call v a box variable if it is defined at the vertices of cells. For our purpose the importance in employing box variables lies in the fact that any average value of a function taken over either a cell volume, a face, or an edge of a cell can be approximated in terms of box variables by means of the trapezoidal rule. Certain other properties to be described then provide a finite difference calculus by means of which summation by parts leads to results similar to those established in Section A.

We employ the notation: v^i indicates the centered average and $v_{,i}$ the centered divided difference with respect to x_i, i.e.,

(C.1.1)
$$v^i = \left(v\left(x_i+\Delta x_i/2\right)+v\left(x_i-\Delta x_i/2\right)\right)/2$$
$$v_{,i} = \left(v\left(x_i+\Delta x_i/2\right)-v\left(x_i-\Delta x_i/2\right)\right)/\Delta x_i \ .$$

For smooth v, therefore,

(C.1.2)
$$v^i = \left(\int_{x_i-\Delta x_i/2}^{x_i+\Delta x_i/2} v(x)dx\right) \div \Delta x_i + O\left(\Delta x_i^2\right);$$

in particular,

$$v^{ij}{}_{,k} = \left(\int_{\pi} \partial_k v dx_i dx_j dx_k\right)/\Delta\pi + O(h^2) \tag{C.1.3}$$

where $\Delta\pi = \Delta x_1 \Delta x_2 \Delta x_3$ and $h = \min\{\Delta x_i\}$.

The algebraic identity

$$(vw)_{,i} = v^i w_{,i} + w^i v_{,i} \tag{C.1.4}$$

then yields a summation by parts formula while the definition

$$v_{,ij} = \left[v(x_i+\Delta x_i/2, x_j+\Delta x_j/2) + v(x_i-\Delta x_i/2, x_j-\Delta x_j/2) - v(x_i-\Delta x_i/2, x_j+\Delta x_j/2)\right.$$
$$\left. - v(x_i+\Delta x_i/2, x_j-\Delta x_j/2)\right] \div (\Delta x_i \Delta x_j)$$

shows that

$$v_{,ij} = v_{,ji}. \tag{C.1.5}$$

The definitions

$$\begin{aligned} \mathrm{div}_h \underline{u} &\equiv \sum_{i=1}^{3} u^{jk}_{i,i} \\ \mathrm{curl}_h \underline{u} &\equiv \left(u^{ij}_{,k} \quad -u^{ik}_{,j}\right) \qquad (ijk) \end{aligned} \tag{C.1.6}$$

provide finite volume approximations to $\mathrm{div}\underline{u}$ and $\mathrm{curl}\underline{u}$ respectively, i.e.,

$$\begin{aligned} \mathrm{div}_h \underline{u} &= \left(\int_p \mathrm{div}\underline{u} d\pi\right) \div \Delta\pi + O(h^2) \\ \mathrm{curl}_h \underline{u} &= \left(\int_\pi \mathrm{curl}\underline{u} \delta\pi\right) \div \Delta\pi + O(h^2). \end{aligned} \tag{C.1.7}$$

We propose to examine the finite difference approximations to (1) given, in terms of box variables in a cell, by

$$\left.\begin{aligned} \operatorname{div}_h \underline{u} &= \rho^{ijk} \\ \operatorname{curl}_h \underline{u} &= \underline{\zeta}^{ijk} \end{aligned}\right\} \qquad (ijk) \tag{C.1.8a}$$

The boundary conditions $\underline{u}\cdot\underline{n} = 0$ are imposed by

$$\underline{u}^{ij}\cdot\underline{n}_k = 0 \qquad (ijk) \tag{C.1.8b}$$

where $\underline{u}^{ij}$ is the trapezoidal approximation to the average value of u on a face σ_k whose normal is $\underline{n}_k$. When box variables are understood we shall often write $\underline{u}\cdot\underline{n} = 0$ to mean the condition expressed by (C.1.8b).

C2. A Summation Identity

Define, using box variables,

$$\begin{aligned} L_h\underline{u} &\equiv A_1\underline{u}^{23}_{,1} + A_2\underline{u}^{13}_{,2} + A_3\underline{u}^{12}_{,3}, \\ \underline{f}_h &\equiv \left(\rho^{123}, \underline{\zeta}^{123}\right) \end{aligned} \tag{C.2.1}$$

where the coefficient matrices are the same as in the definition of $L\underline{u}$ in (A.1.1). The box-variables scheme (C.1.8) expressing $\operatorname{div}\underline{u} = \rho$, $\operatorname{curl}\underline{u} = \underline{\zeta}$ may then be written as

(C.2.2) $$L_h \underline{u} = \underline{f}_h.$$

Next, define

$$\text{grad}_h \underline{u} \equiv \left(\underline{u}^{23}_{,1}, \underline{u}^{13}_{,2}, \underline{u}^{12}_{,3}\right)$$

and

(C.2.3) $$(\underline{u},\underline{v})^h \equiv \left(\text{grad}_h \underline{u} : \text{grad}_h \underline{v}\right).$$

The summation-by-parts formula (C.1.4) then leads to

(C.2.4) $$\left(L_h \underline{u}\right)^T \left(L_h \underline{v}\right) = (\underline{u},\underline{v})^h + \text{div}_h \underline{q}^h - \Omega_h(\underline{u})\underline{v}^h$$

where $\underline{q}^h$ is the vector with components

(C.2.5) $$q_i^h = \left(B_k^T \underline{u}^k_{,j} + B_j \underline{u}^j_{,k}\right)^T \underline{v}^{ik}, \quad (ijk)$$

and

$$\Omega_h \underline{v}^h = \sum_{i=1}^{3} \left(B_k \underline{u}^k_{,ij} + B_k^T \underline{u}^k_{,ji}\right) \underline{v}^{ijk}, \quad (ijk).$$

Since $\underline{u}$ is a box-variable $\underline{u}^k_{,ij} = \underline{u}^k_{,ji}$ ((C.1.5)) and, since $B_k^T = -B_k$, then $\Omega_h \underline{v}^h = 0$.

Next, multiply (C.2.4) by $\Delta\pi$ and sum over D using the summation analogue of Gauss' theorem to obtain

(C.2.6) $$\sum_D \left(L_h \underline{u}\right)^T L_h \underline{v} \Delta\pi = \sum_D (\underline{u},\underline{v})^h \Delta\pi + \sum_\Gamma \underline{q}^h \cdot \underline{n} \Delta\pi.$$

By expressing $\underline{q}^h$ as given by (C.2.5) in terms of the components of $\underline{u}$ and $\underline{v}$ (as in (A.1.7)) the reader may verify that the boundary contribution vanishes when $\underline{u} \cdot \underline{n} = \underline{v} \cdot \underline{n} = 0$ on Γ.

Hence, defining

$$a_h(\underline{u},\underline{v}) \equiv \sum_{D_h} (\underline{u},\underline{v})^h \Delta\pi \tag{C.2.7}$$

we may state: for any box-variables $\underline{u}$ and $\underline{v}$ satisfying (C.1.8b), i.e., $\underline{u}\cdot\underline{n} = \underline{v}\cdot\underline{n} = 0$ on Γ,

$$a_h(\underline{u},\underline{v}) = \sum_D (L_h\underline{u})^T L_h\underline{v}\Delta\pi. \tag{C.2.8}$$

C3. A Convergence Estimate

The box-scheme (C.2.2) is an overdetermined system of algebraic equations under the boundary conditions $\underline{u}\cdot\underline{n} = 0$ on Γ. Consider a solution $\underline{u}^h$ as determined by the least squares problem

$$\min_{u} \sum_D (L_h\underline{u}-\underline{f}_h)^T (L_h\underline{u}-\underline{f}_h)\Delta\pi \tag{C.3.1}$$

with $\underline{u}\cdot\underline{n} = 0$ on Γ.

Using (C.2.8) the Euler equations arising from this problem leads to: $\underline{u}^h$ provides a least-square solution of $L_h\underline{u} = \underline{f}_h$ if

$$a_h(\underline{u}^h,\underline{v}) = \sum_D \underline{f}_h^T L_h\underline{v}\Delta\pi \tag{C.3.2}$$

for any box-variable $\underline{v}$ satisfying $\underline{v}\cdot\underline{n} = 0$. Write

$$\|\underline{u}^h\|^h \equiv (a_h(\underline{u}^h,\underline{u}^h))^{1/2}. \tag{C.3.3}$$

Since only central averages and differences are involved in the definition of $L_h\underline{u}$ it follows that if $\underline{u}$ is a solution of $L\underline{u} = \underline{f}$ which has continuous and bounded mixed third derivatives then $L_h(\underline{u}-\underline{u}^h) = O(h^2)$, i.e.

(C.3.4) $$\|\underline{u}-\underline{u}^h\|^h = O(h^2).$$

Define

(C.3.5) $$\|\underline{u}\|_0^h = \Big[\sum_{\pi\in D}\ \sum_{\sigma\in\pi} \underline{u}^T(\sigma)\underline{u}(\sigma)\Big]^{1/2}$$

where $\underline{u}(\sigma)$ indicates the box-variable approximation to the average value of $\underline{u}$ over a face σ of a cell π. For the continuous problem Friedrichs' inequality, when $\underline{u}\cdot\underline{n} = 0$, yields

$$\|\underline{u}\|_0 \leq \gamma\|\underline{u}\|$$

for some constant γ. The same argument which establishes this inequality may also be followed using summation and difference operators in place of integration and differential operators. The result is

(C.3.6) $$\|\underline{u}\|_0^h \leq \gamma\|\underline{u}\|^h.$$

Using (C.3.4) we thus obtain

$$\|\underline{u}-\underline{u}^h\|_0^h = O(h^2),$$

i.e. the box-scheme is second order accurate in the $\|\cdot\|_0^h$ norm.

C4. A Remark About More General Cells

As indicated earlier the definitions of $\mathrm{div}_h\underline{u}$, $\mathrm{curl}_h\underline{u}$ can be made independent of any assumption about the shape of a cell π. Properly interpreted, so also can the summation by parts formula (C.1.4) as well as (C.1.5). A little reflection will convince the reader that the convergence proof just given applies as well for irregularly shaped subdomains.

The followng describes explicit representations for the box-scheme on irregular cells.

Let σ_ν denote an oriented face of $\pi, \nu = 1,2,\dots,6$. Applying (C.1.7) to a smooth function $\underline{u}$, and employing Gauss' theorem,

$$\Delta\pi\cdot\mathrm{div}_h\underline{u} \simeq \int_\pi \mathrm{div}\underline{u}\,d\pi = \sum_\nu \int_{\sigma_\nu} \underline{u}\cdot d\underline{\sigma} \simeq \hat{\underline{u}}(\underline{\sigma}_\nu)\cdot\Delta\underline{\sigma}_\nu \tag{C.4.1}$$

where $\hat{\underline{u}}(\underline{\sigma}_\nu)$ indicates the value of $\underline{u}$ at the centroid of $\underline{\sigma}_\nu$. By approximating $\hat{\underline{u}}(\underline{\sigma}_\nu)$ by the average of its values at the vertex points of $\underline{\sigma}_\nu$ an expresison for $\mathrm{div}_h\underline{u}$ results when $\underline{u}$ is a box-variable.

Similarly,

$$\mathrm{curl}_h\underline{u}\cdot\underline{n}_i \simeq \int_\pi (\mathrm{curl}\underline{u}\cdot\underline{n}_i)\,d\pi/\Delta\pi .$$

Apply Stoke's theorem on a face $d\underline{\sigma}_\nu$ and let $d\underline{s}_\nu$ indicate an element of arc length in the direction $\underline{t}_{\nu i} = d\underline{\sigma}_\nu x\underline{n}_i$; the result is

$$\mathrm{curl}_h\underline{u}\cdot\underline{n}_i \simeq \sum_\nu \int_{\sigma_\nu} (\underline{u}\cdot\underline{t}_{\nu i})\,ds_\nu dx_i/\Delta\pi \simeq \sum_\nu (\underline{u}\cdot\underline{t}_{\nu i})\Delta\sigma_\nu/\Delta\pi \tag{C.4.2}$$

where $\underline{u}\cdot\underline{t}_{\nu i}$ is evaluated at the centroid of the face $\underline{\sigma}_\nu$ having the area $\Delta\sigma_\nu$. By evaluating $\underline{u}\cdot\underline{t}_{\nu i}$ as the average of its values at the vertices of $\underline{\sigma}_\nu$ (C.4.2) provides an interpretation of $\mathrm{curl}_h\underline{u}$ in terms of box-variables.

Concluding Remarks

A comparison of the convergence proofs employed in Parts B and C is of interest. The finite-element approach allowed the integral identity (A.1.9) to be used directly but utilized estimates arising from the adjoint problem. The finite difference approach, on the other hand, required the development of a summation identity corresponding to (A.1.9); Friedrichs′ inequality then provided in the required convergence estimate.

Both proofs are independent of any assumptions about the type of cells π upon which approximations are based. However, the numerical implementation of the finite-element approach in such cases may be simpler to employ than the box-scheme because of extensive and readily available software for finite-element methods. The above remarks suggest that this software could be adapted to the finite difference method as well.

Both methods lead to sparse matrices which may be solved by direct algebraic techniques. An iterative scheme for least squares problems due to Kaczmarz [6] and Tanabe [11] provides an alternative approach and has been employed in [4] to treat the finite difference problem in two dimensions. Progress in developing fast iterative methods has been reported to us in personal communictions by our colleagues (Grosch and Phillips) and will be described elsewhere.

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16 Abstract

A least squares formulation of the system $\mathrm{div}\,\underline{u} = \rho$, $\mathrm{curl}\,\underline{u} = \underline{\zeta}$ is surveyed from the viewpoint of both finite element and finite difference methods. Closely related arguments are shown to establish convergence estimates.

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