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UNCOUPLED FINITE ELEMENT SOLUTION OF BIHARMONIC PROBLEMS FOR VECTOR POTENTIALS

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SUMMARY

A method for the uncoupled solution of three-dimensional biharmonic problems for the vector potential in viscous incompressible flow is presented. The strategy applied in a previous work on vector Poisson equations is employed to reduce the vector fourth-order problem to a sequence of scalar biharmonic problems. A finite element aimed at the implementation of the method in a discrete version is considered. A conjugate gradient algorithm which is particularly efficient for the uncoupled solution method is also described.

1. INTRODUCTION

In the study of two-dimensional viscous incompressible flows, the formulation based on the streamfunction and the biharmonic equation is attractive since one has to deal with only one scalar unknown. A detailed discussion of this formulation can be found in Reference 1, while efficient methods for the numerical solution are proposed in Reference 2.

The analogous formulation for the three-dimensional case is based on the vector potential, also called the stream vector, the curl of which is the velocity field of the fluid. However, except for the case of axisymmetric flows, one cannot expect to obtain a simple solution method, not even for the Stokes problem, since the three Cartesian components of the vector potential are strongly coupled through the boundary conditions (see e.g. Reference 3).

Indeed, in order to attain a simplification comparable to the streamfunction, one should be able to express the Stokes problem at the very outset in the form of three independent biharmonic equations for the components of the vector unknown. In this work we present instead a method which enables one to transform the coupled biharmonic system for the vector potential into a fast-converging sequence of scalar biharmonic problems supplemented with non-homogeneous Dirichlet boundary conditions. This assertion is supported by numerical results obtained in Reference 4 using a finite element discretization proposed in Reference 5. Fast convergence is achieved by implementing the uncoupling technique via the conjugate gradient algorithm, similarly to a method recently proposed for the decoupled solution of vector Poisson equations with the divergence of the unknown prescribed on the boundary.[6]

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The outline of the paper is as follows. After introducing the problem to solve in Section 2, in Section 3 we present the uncoupling technique for the continuous problem in a formal way. In Section 4 we consider a finite element method suitable for the discretization of the so-obtained decoupled formulation of the problem. Next we give in Section 5 an algorithm of the conjugate gradient type which is particularly handy for the discrete form of the proposed formulation. We conclude in Section 6 with some remarks.

2. THE STOKES PROBLEM IN TERMS OF THE VECTOR POTENTIAL

In order to describe the uncoupling method in connection with the boundary conditions for the vector potential, it suffices to consider a stationary Stokes problem in a star-shaped bounded domain $\Omega \subset \mathbb{R}^3$ with boundary Γ, namely

$$\begin{aligned} -\nu\Delta\mathbf{u} + \nabla p &= \mathbf{f}, \\ \nabla\cdot\mathbf{u} &= 0, \\ \mathbf{u}|_\Gamma &= \mathbf{b}, \end{aligned} \tag{1}$$

where $\mathbf{u}$ is the velocity field and p is the hydrostatic pressure, defined up to an additive constant. Furthermore, ν is the coefficient of kinematic viscosity, $\mathbf{f}$ represents body forces and $\mathbf{b}$ denotes the velocity prescribed on Γ. The boundary datum $\mathbf{b}$ is assumed to satisfy the global condition $\int \mathbf{n}\cdot\mathbf{b}\,d\Gamma = 0$, where $\mathbf{n}$ denotes the outer unit normal vector with respect to Γ. Although this is by no means essential, to simplify the presentation we shall assume that $\mathbf{f}$, $\mathbf{b}$ and Γ are smooth enough to yield desirably smooth solutions.

Since $\mathbf{u}$ is divergence-free, there exists a *vector potential* $\boldsymbol{\psi}$ such that

$$\nabla \times \boldsymbol{\psi} = \mathbf{u}.$$

Of course, $\boldsymbol{\psi}$ is defined only up to an additive gradient, say $\nabla\theta$. Thus, assigning appropriately the value of $\Delta\theta$, we can further require that $\boldsymbol{\psi}$ be divergence-free, i.e $\nabla\cdot\boldsymbol{\psi} = 0$ (Euclidean gauge). This condition still leaves $\boldsymbol{\psi}$ defined up to the gradient of a harmonic function and can be enforced simply by imposing the boundary condition

$$\nabla\cdot\boldsymbol{\psi}|_\Gamma = 0. \tag{2}$$

Apart from such a boundary condition, we must consider the boundary conditions induced by the original specification of velocity on the boundary, namely

$$\nabla \times \boldsymbol{\psi}|_\Gamma = \mathbf{b}$$

or, expressing the normal and tangential components separately,

$$\mathbf{n}\cdot\nabla\times\boldsymbol{\psi}|_\Gamma = \mathbf{n}\cdot\mathbf{b} \quad \text{and} \quad \mathbf{n}\times\nabla\times\boldsymbol{\psi}|_\Gamma = \mathbf{n}\times\mathbf{b}.$$

Now we can take full advantage of the remaining arbitrariness of $\boldsymbol{\psi}$ by the gradient of a harmonic function, in order to transform the normal component of the boundary condition for $\nabla\times\boldsymbol{\psi}$ into a boundary condition for the tangential components of $\boldsymbol{\psi}$, in the form

$$\mathbf{n}\times\boldsymbol{\psi}|_\Gamma = \mathbf{n}\times\mathbf{a}, \tag{3}$$

where the tangential vector field $\mathbf{a}$ on the boundary is obtained from the datum $\mathbf{n}\cdot\mathbf{b}$ through the solution of a scalar elliptic problem over the boundary (Beltrami problem).[7] The tangential part of the velocity boundary condition is instead retained in its original form, namely

$$\mathbf{n}\times\nabla\times\boldsymbol{\psi}|_\Gamma = \mathbf{n}\times\mathbf{b}. \tag{4}$$

Let us now take the curl of the first equation in (1) to obtain the equation

$$-\nu\nabla\times[\Delta(\nabla\times\boldsymbol{\psi})]=\nabla\times\mathbf{f}$$

or, using the vector identity $\nabla\times\nabla\times\ldots=-\Delta\ldots+\nabla(\nabla\cdot\ldots)$, the equivalent equation

$$\nu[\Delta^2\boldsymbol{\psi}-\Delta\nabla(\nabla\cdot\boldsymbol{\psi})]=\nabla\times\mathbf{f}.$$

Thus, if we are able to set suitable conditions on $\boldsymbol{\psi}$, we can assert that $\boldsymbol{\psi}$ verifies

$$\nu\Delta^2\boldsymbol{\psi}=\nabla\times\mathbf{f} \tag{5}$$

plus the boundary conditions (2)–(4). We have in fact five independent boundary conditions for $\boldsymbol{\psi}$ and the missing one can be chosen so that the term $\Delta[\nabla(\nabla\cdot\boldsymbol{\psi})]$ vanishes. Two possibilities arise quite naturally in this connection, namely $\mathbf{n}\cdot\nabla(\nabla\cdot\boldsymbol{\psi})|_\Gamma=0$ and $\Delta(\nabla\cdot\boldsymbol{\psi})|_\Gamma=0$. Actually, adding either of these two boundary conditions to (2)–(5), one can establish the equivalence between the resulting system and (1) through the relation $\nabla\times\boldsymbol{\psi}=\mathbf{u}$, for a suitable pressure field. In this work, for technical reasons to be specified below, we will select the second natural boundary condition

$$[\Delta(\nabla\cdot\boldsymbol{\psi})]\,|_\Gamma=0. \tag{6}$$

As has been proved in Reference 3, the vector potential defined by (2)–(6) is the unique solution to the following variational problem:

$$\left.\begin{aligned}&\text{find } \boldsymbol{\psi}\in\mathbf{H}^2(\Omega) \text{ such that } \mathbf{n}\times\boldsymbol{\psi}|_\Gamma=\mathbf{n}\times\mathbf{a},\ \mathbf{n}\times\nabla\times\boldsymbol{\psi}|_\Gamma=\mathbf{n}\times\mathbf{b},\ \nabla\cdot\boldsymbol{\psi}|_\Gamma=0,\\ &\nu\int_\Omega\Delta\boldsymbol{\psi}\cdot\Delta\boldsymbol{\phi}=\int_\Omega\nabla\times\mathbf{f}\cdot\boldsymbol{\phi},\quad\forall\boldsymbol{\phi}\in\mathbf{X},\end{aligned}\right\} \tag{7}$$

where*

$$\mathbf{X}=\{\boldsymbol{\phi}\,|\,\boldsymbol{\phi}\in\mathbf{H}^2(\Omega),\quad\mathbf{n}\times\boldsymbol{\phi}|_\Gamma=\mathbf{0},\quad\mathbf{n}\times\nabla\times\boldsymbol{\phi}|_\Gamma=\mathbf{0},\quad\nabla\cdot\boldsymbol{\phi}|_\Gamma=0\}.$$

This is the reason for selecting condition (6), since problem (7) is a very convenient formulation in view of a decoupled solution method. Indeed, the coupling of the three components of $\boldsymbol{\psi}$ is due only to the boundary conditions implicit in space $\mathbf{X}$. Actually, if we were assigned an additional essential boundary condition, namely

$$n\cdot\boldsymbol{\psi}|_\Gamma=\lambda, \tag{8}$$

problem (7) would simply become a (decoupled) set of three scalar biharmonic problems, i.e.

$$\left.\begin{aligned}&\text{find } \psi_i\in H^2(\Omega) \text{ such that } \psi_i|_\Gamma=\alpha_i,\quad\partial\psi_i/\partial n|_\Gamma=\beta_i,\\ &\nu\int_\Omega\Delta\psi_i\Delta\phi=\int_\Omega g_i\phi,\quad\forall\phi\in H_0^2(\Omega),\quad i=1,2,3,\end{aligned}\right\} \tag{9}$$

where the boundary functions α_i and β_i are derived from $\mathbf{a}$, $\mathbf{b}$ and λ by a straightforward calculation and $g_i\equiv(\nabla\times\mathbf{f})_i$. Of course, if this is so, we must obtain λ from the natural boundary condition (6), which was not explicitly taken into account in (9). A way of performing this is described in the following section.

3. DETERMINING THE VALUES FOR THE MISSING ESSENTIAL BOUNDARY CONDITION

Following the usual procedure in the influence matrix technique, we first write $\boldsymbol{\psi}$ as

$$\boldsymbol{\psi}(\mathbf{x})=\boldsymbol{\psi}_0(\mathbf{x})+\langle\boldsymbol{\psi}_\mathbf{s}(\mathbf{x}),\lambda(\mathbf{s})\rangle_{3/2,\mathbf{s}},\quad\forall\mathbf{x}\in\bar{\Omega}, \tag{10}$$

*See Reference 8 for definitions of Sobolev spaces $\mathbf{H}^s(D)$, $D\subset\mathbb{R}^n$, $s\in\mathbb{R}$.

where $\langle .,. \rangle_{3/2,\mathbf{s}}$ denotes the duality product between $H^{-3/2}(\Gamma)$ and $H^{3/2}(\Gamma)$, with $\mathbf{s}$ taken as the independent variable on Γ. The field $\boldsymbol{\psi}_0$ belongs to $\mathbf{H}^2(\Omega)$ and verifies

$$\nu\Delta^2\boldsymbol{\psi}_0 = \nabla\times\mathbf{f}, \tag{11}$$

$$\mathbf{n}\cdot\boldsymbol{\psi}_0|_\Gamma = 0, \qquad \mathbf{n}\times\boldsymbol{\psi}_0|_\Gamma = \mathbf{n}\times\mathbf{a},$$

$$\nabla\cdot\boldsymbol{\psi}_0|_\Gamma = 0, \qquad \mathbf{n}\times\nabla\times\boldsymbol{\psi}_0|_\Gamma = \mathbf{n}\times\mathbf{b}. \tag{11a}$$

On the other hand, the field $\boldsymbol{\psi}_s$, $\forall\mathbf{s}\in\Gamma$, is a distribution in the topological dual space of $\mathbf{H}^1(\Omega)$ and is defined as follows:

$$\nabla\times\boldsymbol{\psi}_\mathbf{s}\in\mathbf{H}(\mathrm{curl},\Omega) \equiv \{\boldsymbol{\phi}\,|\,\boldsymbol{\phi}\in\mathbf{L}^2(\Omega),\quad \nabla\times\boldsymbol{\phi}\in\mathbf{L}^2(\Omega)\},$$

$$\nabla\cdot\boldsymbol{\psi}_\mathbf{s}\in H_0^1(\Omega) \equiv \{v|v\in H^1(\Omega),\qquad v|_\Gamma = 0\}, \tag{12}$$

$$\mathbf{n}\times\boldsymbol{\psi}_\mathbf{s}|_\Gamma = \mathbf{0}\quad(\text{in }\mathbf{H}^{-3/2}(\Gamma)),\qquad \mathbf{n}\times\nabla\times\boldsymbol{\psi}_\mathbf{s}|_\Gamma = \mathbf{0}\quad(\text{in }\mathbf{H}^{-1/2}(\Gamma)), \tag{13}$$

$$\int_\Omega \nabla\times\nabla\times\boldsymbol{\psi}_\mathbf{s}\cdot\nabla\times\nabla\times\boldsymbol{\phi} + \int_\Omega \nabla(\nabla\cdot\boldsymbol{\psi}_\mathbf{s})\cdot\nabla(\nabla\cdot\boldsymbol{\phi}) = \Delta(\nabla\cdot\boldsymbol{\phi})(\mathbf{s}),\quad \forall\boldsymbol{\phi}\in\mathbf{H}^5(\Omega). \tag{14}$$

Using standard arguments, one can prove that such a field $\boldsymbol{\psi}_\mathbf{s}$, besides the boundary conditions implicit in (12) and (13), satisfies

$$\Delta^2\boldsymbol{\psi}_\mathbf{s} = \mathbf{0}\quad(\text{in }\mathbf{H}^{-5}(\Omega)). \tag{15}$$

Moreover, since $\forall\xi\in H^{3/2}(\Gamma)$, it is possible to find (a unique) $\boldsymbol{\phi}\in\mathbf{H}^5(\Omega)$ such that

$$\nu\Delta^2\boldsymbol{\phi} = \mathbf{0},$$

$$[\Delta(\nabla\cdot\boldsymbol{\phi})]|_\Gamma = \xi, \qquad \mathbf{n}\times\boldsymbol{\phi}|_\Gamma = \mathbf{0},$$

$$\nabla\cdot\boldsymbol{\phi}|_\Gamma = 0, \qquad \mathbf{n}\times\nabla\times\boldsymbol{\phi}|_\Gamma = \mathbf{0},$$

by applying Green's formulae to (14) one can easily check that $\boldsymbol{\psi}_\mathbf{s}$ also satisfies

$$\langle\mathbf{n}\cdot\boldsymbol{\psi}_\mathbf{s},\xi\rangle_{3/2,\Gamma} = \xi(\mathbf{s}),\quad \forall\xi\in H^{3/2}(\Gamma), \tag{16}$$

where $\langle .,. \rangle_{3/2,\Gamma}$ denotes the duality product between $H^{-3/2}(\Gamma)$ and $H^{3/2}(\Gamma)$, s being now a fixed point of Γ.

Remark 1. Perhaps a simpler way of interpreting equation (16) is as

$$\mathbf{n}\cdot\boldsymbol{\psi}_\mathbf{s}|_\Gamma = \delta^{(2)}(\boldsymbol{\sigma}-\mathbf{s})\quad\text{in}\quad H^{-3/2}(\Gamma),$$

where $\delta^{(2)}(\boldsymbol{\sigma})$ is the surface Dirac distribution.

We do not address here the question of the existence and uniqueness of $\boldsymbol{\psi}_\mathbf{s}$. However, we can state that, although $\boldsymbol{\psi}_\mathbf{s}$ is not even a field of $\mathbf{L}^2(\Omega)$ in general, by construction $\langle\boldsymbol{\psi}_\mathbf{s},\lambda(\mathbf{s})\rangle_{3/2,\mathbf{s}}\in\mathbf{H}^2(\Omega)$. In fact, we shall assume henceforth the same required smoothness for $\boldsymbol{\psi}$ and $\boldsymbol{\psi}_0$, which will consequently apply to $\langle\boldsymbol{\psi}_\mathbf{s},\lambda(\mathbf{s})\rangle_{3/2,\mathbf{s}}$ as well.

Anyhow, the point to be stressed for our purpose is the fact that, $\forall\mathbf{s}\in\Gamma$, $\boldsymbol{\psi}_\mathbf{s}$ can be determined by solving three decoupled scalar biharmonic problems with (singular) non-homogeneous Dirichlet conditions, which are formally defined by (12), (13), (16) together with a variational form associated with biharmonic equation (15), namely

$$\int_\Omega \nabla\times\nabla\times\boldsymbol{\psi}_\mathbf{s}\cdot\nabla\times\nabla\times\boldsymbol{\phi} + \int_\Omega \nabla(\nabla\cdot\boldsymbol{\psi}_\mathbf{s})\cdot\nabla(\nabla\cdot\boldsymbol{\phi}) = 0,\quad \forall\boldsymbol{\phi}\in\mathbf{H}_0^2(\Omega). \tag{17}$$

As a matter of fact, using the identity

$$\nabla \times \nabla \times \ldots = -\Delta \ldots + \nabla(\nabla \cdot \ldots), \tag{18}$$

it is straightforward to conclude that (15) is equivalent to the (uncoupled) vector biharmonic problem

$$\int_\Omega \Delta \boldsymbol{\psi}_s \cdot \Delta \boldsymbol{\phi} = 0, \quad \forall \boldsymbol{\phi} \in \mathbf{H}_0^2(\Omega).$$

Now, recalling (10) and the natural boundary condition (6), and the assumption that the data are smooth enough, we can write

$$[\Delta(\nabla \cdot \boldsymbol{\psi}_0(\mathbf{x})) + \Delta \nabla \cdot \langle \boldsymbol{\psi}_s(\mathbf{x}), \lambda(\mathbf{s}) \rangle_{3/2,s}]|_\Gamma = 0.$$

Next we apply the duality product with $\mathbf{n} \cdot \boldsymbol{\psi}_{s'}$, $s' \in \Gamma$, thereby obtaining

$$\langle \mathbf{n} \cdot \boldsymbol{\psi}_{s'}, \Delta(\nabla \cdot \boldsymbol{\psi}_0) \rangle_{3/2,\Gamma} + \langle \mathbf{n} \cdot \boldsymbol{\psi}_{s'}, \Delta \nabla \cdot \langle \boldsymbol{\psi}_s, \lambda(\mathbf{s}) \rangle_{3/2,s} \rangle_{3/2,\Gamma} = 0.$$

However, by definition we have

$$\langle \mathbf{n} \cdot \boldsymbol{\psi}_{s'}, \Delta(\nabla \cdot \boldsymbol{\psi}_0) \rangle_{3/2,\Gamma} = \int_\Omega (\nabla \cdot \boldsymbol{\psi}_{s'}) \Delta(\nabla \cdot \boldsymbol{\psi}_0) + \langle \boldsymbol{\psi}_{s'}, \nabla \Delta(\nabla \cdot \boldsymbol{\psi}_0) \rangle_{1,\Omega},$$

where $\langle \cdot, \cdot \rangle_{m,\Omega}$ denotes the duality product between $\mathbf{H}^m(\Omega)$ and its dual. Moreover, using identity (18) reiterately, we have

$$\Delta^2 \ldots = \nabla \times \nabla \times \nabla \times \nabla \times \ldots + \nabla(\nabla \cdot \Delta \ldots), \tag{19}$$

which yields

$$\langle \boldsymbol{\psi}_{s'}, \nabla \Delta(\nabla \cdot \boldsymbol{\psi}_0) \rangle_{1,\Omega} = \langle \boldsymbol{\psi}_{s'}, \nabla \times (\nu^{-1} \mathbf{f} - \nabla \times \nabla \times \nabla \times \boldsymbol{\psi}_0) \rangle_{1,\Omega}$$

or, using (12), (13) and Green's formulae.

$$\langle \mathbf{n} \cdot \boldsymbol{\psi}_{s'}, \Delta(\nabla \cdot \boldsymbol{\psi}_0) \rangle_{3/2,\Gamma} = \nu^{-1} \int_\Omega \nabla \times \mathbf{f} \cdot \boldsymbol{\psi}_{s'} - a(\boldsymbol{\psi}_{s'}, \boldsymbol{\psi}_0), \tag{20}$$

where for every pair of fields $\boldsymbol{\psi}$, $\boldsymbol{\phi}$ belonging to the spaces specified in (12), (13) we set

$$a(\boldsymbol{\psi}, \boldsymbol{\phi}) = \int_\Omega \nabla \times \nabla \times \boldsymbol{\psi} \cdot \nabla \times \nabla \times \boldsymbol{\phi} + \int_\Omega \nabla(\nabla \cdot \boldsymbol{\psi}) \cdot \nabla(\nabla \cdot \boldsymbol{\phi}). \tag{21}$$

In fact, (20) was derived by exploiting again the boundary conditions for $\boldsymbol{\psi}_{s'}$ and the assumed smoothness of $\boldsymbol{\psi}_0$. Analogously we have

$$\langle \mathbf{n} \cdot \boldsymbol{\psi}_{s'}, \Delta \nabla \cdot \langle \boldsymbol{\psi}_{s'}, \lambda(\mathbf{s}) \rangle_{3/2,s} \rangle_{3/2,\Gamma} = \langle \boldsymbol{\psi}_{s'}, \nabla \Delta \nabla \cdot \langle \boldsymbol{\psi}_{s'}, \lambda(\mathbf{s}) \rangle_{3/2,s} \rangle_{1,\Omega} + \int_\Omega \nabla \cdot \boldsymbol{\psi}_{s'} \Delta \nabla \cdot \langle \boldsymbol{\psi}_s, \lambda(\mathbf{s}) \rangle_{3/2,s}.$$

Since $\Delta^2 \boldsymbol{\psi}_s = \mathbf{0}$, $\forall s \in \Gamma$, from identity (19) and an argument already employed in (20), we obtain

$$\langle \mathbf{n} \cdot \boldsymbol{\psi}_{s'}, \Delta \nabla \cdot \langle \boldsymbol{\psi}_s, \lambda(\mathbf{s}) \rangle_{3/2,s} \rangle_{3/2,\Gamma} = -a(\boldsymbol{\psi}_{s'}, \langle \boldsymbol{\psi}_s, \lambda(\mathbf{s}) \rangle_{3/2,s}). \tag{22}$$

As a conclusion, the unknown λ can be determined by solving the following problem:

$$a(\boldsymbol{\psi}_{s'}, \langle \boldsymbol{\psi}_s, \lambda(\mathbf{s}) \rangle_{3/2,s}) = \nu^{-1} \int_\Omega \nabla \times \mathbf{f} \cdot \boldsymbol{\psi}_{s'} - a(\boldsymbol{\psi}_{s'}, \boldsymbol{\psi}_0), \quad \forall s' \in \Gamma. \tag{23}$$

Remark 2. As a matter of fact, for a given $\mathbf{x} \in \Omega$, $\psi_{\mathbf{s}}(\mathbf{x})$ depends continuously on $\mathbf{s}$ for a smooth domain, so that we can actually write

$$\langle \psi_{\mathbf{s}}(\mathbf{x}), \lambda(\mathbf{s}) \rangle_{3/2,\mathbf{s}} = \int_\Gamma \hat{\psi}(\mathbf{x}, \mathbf{s}) \lambda(\mathbf{s}) \, d\mathbf{s},$$

where $\hat{\psi}(\mathbf{x}, \mathbf{s}) \equiv \psi_{\mathbf{s}}(\mathbf{x})$, $\forall \mathbf{s} \in \Gamma$, $\forall \mathbf{x} \in \Omega$. Thus, applying Fubini's theorem, problem (23) can also be written as

$$\int_\Gamma a(\hat{\psi}(\cdot, \mathbf{s}'), \hat{\psi}(\cdot, \mathbf{s})) \lambda(\mathbf{s}) \, d\mathbf{s} = \nu^{-1} \int_\Omega \nabla \times \mathbf{f}(\mathbf{x}) \cdot \hat{\psi}(\mathbf{x}, \mathbf{s}') \, d\mathbf{x} - a(\hat{\psi}(\cdot, \mathbf{s}'), \psi_0(\cdot)), \quad \forall \mathbf{s}' \in \Gamma.$$

Remark 3. The left-hand side of (23) corresponds to the influence matrix indexed by $\mathbf{s}$ and $\mathbf{s}'$.

4. FINITE ELEMENT DISCRETIZATION

To implement the method described in the previous section, the basic tool that is needed is an efficient finite element method for solving scalar biharmonic-problems in $\mathbb{R}^3$ of type (9), together with the linear problem (23).

We shall consider here a *non-conforming* quadratic finite element of first order in the energy norm, first introduced in Reference 5. After recalling the precise definition of the element, we will treat some computational aspects pertaining to the specific application we are interested in. In particular, we will define a discrete analogue of the surface Dirac distribution. Moreover, we will describe the way of approximating boundary unknown λ related to this finite element approximation.

Let us be given a family $\{\mathbf{T}_h\}_h$ of tetrahedrizations of Ω, assumed to be quasi-uniform in the usual sense. Here h denotes the maximum edge length of the tetrahedrons belonging to $\mathbf{T}_h$. We assume that $\mathbf{T}_h$ fits Ω in the sense that the intersection of any tetrahedron $T \in \mathbf{T}_h$ with Γ is either empty or coincides with one or more faces, edges or vertices of T.

For each $T \in \mathbf{T}_h$ the quadratic finite element method is defined by the following set of 10 degrees of freedom:

(1) the mean values of the function over each edge
(2) the first-order normal derivatives of the function at the barycentre of each face in a given sense (outwards or inwards).

Here the mean value of a function v over an edge e is to be understood as $\int_e v \, de/|e|$, where $|e|$ denotes the length of e.

Now we define V_h to be the space of (scalar) functions whose restriction to every tetrahedron of $\mathbf{T}_h$ is quadratic and such that the degrees of freedom above coincide at inter-elemental boundaries. We further define $V_{h,0}$ to be the subspace of V_h consisting of those functions whose degrees of freedom vanish whenever the corresponding edge or face is a boundary edge or face. Here a boundary edge means an edge of an element $T \in \mathbf{T}_h$ whose intersection with Γ contains its two end points, and a boundary face means a face of $T \in \mathbf{T}_h$ whose intersection with Γ contains its three vertices.

We also have to define the affine manifold $V_{h,\alpha\beta}$ of V_h in order to take into account the non-homogeneous boundary conditions of problem (9). Let us first denote by $\mathbf{E}_h$ the set of boundary edges and by $\mathbf{F}_h$ the set of boundary faces. The degrees of freedom of a function of $V_{h,\alpha\beta}$ attached to $e \in \mathbf{E}_h$ are defined as follows. Let $F_e^{(1)}$ and $F_e^{(2)}$ be the boundary faces of $T \in \mathbf{T}_h$ whose intersection is e. Referring to Figure 1, we denote by π_e the plane bisecting the dihedron formed by faces $F_e^{(1)}$

and $F_e^{(2)}$ oriented towards the interior of Ω, and by n_e the straight line of π_e orthogonal to e passing through the midpoint of the latter. The degree of freedom attached to each $e \in \mathbf{E}_h$ of a function of $V_{h,\alpha\beta}$ is the value of α at P_e, namely the intersection, lying closest to e, of n_e with Γ (or of n_e with γ_e, where $\gamma_e = \pi_e \cap \Gamma$). As for the normal derivative of a function of $V_{h,\alpha\beta}$ at the barycentre G_F of a face $F \in \mathbf{F}_h$, we define it to be the value of β at the point M_F, namely the intersection with Γ lying closest to F of the perpendicular to F passing through G_F (refer to Figure 2).

Let us now define a discrete analogue of problem (9) associated with the component $\psi_i \equiv \psi$ of the vector potential, namely

$$\left.\begin{aligned} &\text{find } \psi_h \in V_{h,\alpha\beta} \text{ such that} \\ &\tilde{a}_h(\psi_h, \phi_h) = \nu^{-1} \int_{\Omega_h} g\phi_h, \quad \forall \phi_h \in V_{h,0}, \end{aligned}\right\} \tag{24}$$

where g is an appropriate right-hand side ($g = g_i = (\nabla \times \mathbf{f})_i$ in the specific case of problem (7)).

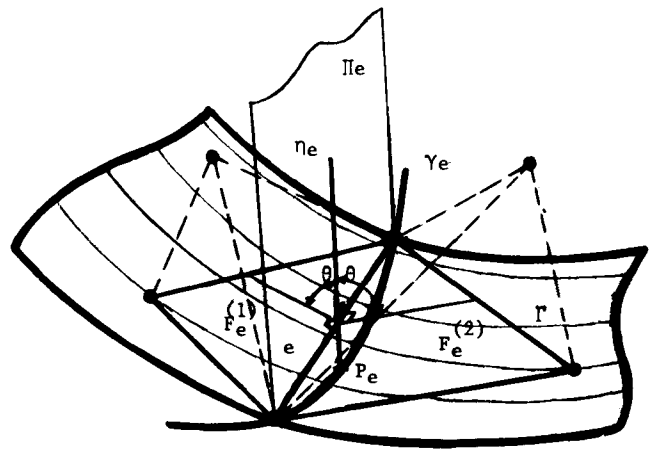

Figure 1. Boundary faces $F_e^{(1)}$ and $F_e^{(2)}$

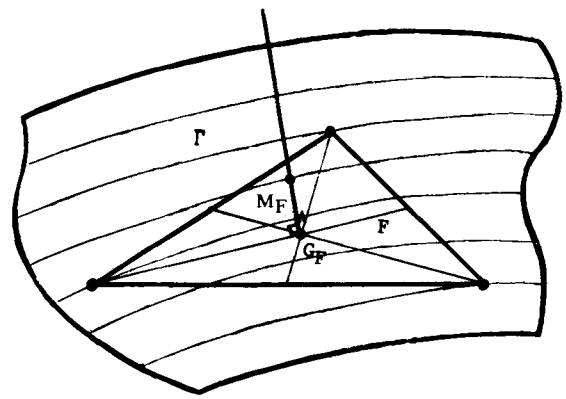

Figure 2. Shifting from $M_F \in \Gamma$ to the barycentre of $F \in \mathbf{F}_h$

Bilinear form $\tilde{a}_h$ is a discrete analogue of $\int_\Omega \Delta\psi\,\Delta\phi$, namely

$$\tilde{a}_h(\psi, \phi) \equiv \sum_{T\in\mathbf{T}_h} \int_T \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial^2\psi}{\partial x_i \partial x_j} \frac{\partial^2\phi}{\partial x_i \partial x_j}, \tag{25}$$

whereas $\Omega_h \equiv \cup_{T\in\mathbf{T}_h} T$.

Remark 4. Note that, $\forall\phi\in H_0^2(\Omega_h)$ and $\forall\psi\in H^2(\Omega_h)$, $\tilde{a}_h(\psi, \phi) = \int_{\Omega_h} \Delta\psi\,\Delta\phi$ (see e.g. Reference 5), but this equivalence is false if $\psi\in V_h$ and $\phi\in V_{h,0}$.

The computation of the approximation ϕ_h to ϕ and of the approximation $\psi_{i,h}$ to ψ_i, $i = 1, 2, 3$ (assuming that λ is known), follows standard and straightforward procedures applied to problem (24). Therefore we choose here to illustrate the use of this problem in the case of the computation of approximations of $\boldsymbol{\psi}_\mathbf{s}$, $\mathbf{s}\in\Gamma$, in $[V_h]^3$.

First of all, in the discrete case, instead of computing for every $\mathbf{s}\in\Gamma$ a discrete analogue of $\boldsymbol{\psi}_\mathbf{s}$, we will select only one point per edge of $\mathbf{E}_h$. In other words, we need only $\boldsymbol{\psi}_{h,e}$, namely an approximation of $\boldsymbol{\psi}_\mathbf{s}$, where $\mathbf{s}$ is the point P_e. Notice that the data α_i and β_i are not really functions in this case, but, as far as the discrete problem is concerned, all that is needed are boundary degrees of freedom of $\mathbf{n}_e\cdot\boldsymbol{\psi}_{h,e}$ which would tend in a reasonable sense to the surface Dirac distribution at a point of Γ as h goes to zero, $\mathbf{n}_e$ being the unit vector in the direction of n_e. The natural way of defining such a degree of freedom is as follows.

Let p_e be the basis function of V_h associated with edge $e\in\mathbf{E}_h$, i.e. $\int_e p_e\,de = |e|$, whereas all of its remaining degrees of freedom vanish. The support of p_e is just the set of tetrahedrons whose intersection is e, and clearly the only boundary faces over which p_e does not vanish identically are $F_e^{(1)}$ and $F_e^{(2)}$. Quite naturally we would then like $\mathbf{n}\cdot\boldsymbol{\psi}_{h,e}$ to verify the condition

$$\int_{F_e^{(1)}\cap F_e^{(2)}} \mathbf{n}_e\cdot\boldsymbol{\psi}_{h,e}\,dF = 1.$$

Thus the degree of freedom d_e of $\mathbf{n}_e\cdot\boldsymbol{\psi}_{h,e}$ attached to e must satisfy

$$d_e = \left(\int_{F_e^{(1)}\cap F_e^{(2)}} p_e\,dF\right)^{-1}, \tag{26}$$

while the remaining edge degrees of freedom of $\boldsymbol{\psi}_{h,e}$ vanish.

However, in order to take into account the boundary condition $\mathbf{n}\times\nabla\times\boldsymbol{\psi}_\mathbf{s}|_\Gamma = \mathbf{0}$, we must compute normal derivative degrees of freedom at the barycentre of both $F_e^{(1)}$ and $F_e^{(2)}$ for the two tangential components of $\boldsymbol{\psi}_{h,e}$ with respect to those faces. Letting $G_e^{(r)}$ be the barycentre of $F_e^{(r)}$, $r = 1, 2$, $\boldsymbol{\tau}_e^{(r)}$ be any unit tangential vector of $F_e^{(r)}$, and $\mathbf{n}_e^{(r)}$ be the unit normal vector with respect to $F_e^{(r)}$, we have

$$\frac{\partial(\boldsymbol{\tau}_e^{(r)}\cdot\boldsymbol{\psi}_{h,e})}{\partial n_e^{(r)}} = \frac{\partial(\mathbf{n}_e^{(r)}\cdot\boldsymbol{\psi}_{h,e})}{\partial\tau_e^{(r)}} \quad \text{at} \quad G_e^{(r)}. \tag{27}$$

Incidentally, all the degrees of freedom of $\mathbf{n}_e^{(r)}\cdot\boldsymbol{\psi}_{h,e}$ associated with edges of $\mathbf{E}_h$ vanish, except for the one associated with e itself, whose value is precisely $d_e^{(r)} = d_e\mathbf{n}_e^{(r)}\cdot\mathbf{n}_e$. On the other hand, according to Reference 5, any tangential derivative of $\mathbf{n}_e^{(r)}\cdot\boldsymbol{\psi}_{h,e}$ at $G_e^{(r)}$ is given by $\alpha(\boldsymbol{\tau}_e^{(r)})\,d_e^{(r)}$, where the coefficient $\alpha(\boldsymbol{\tau}_e^{(r)})$ depends only on face $F_e^{(r)}$ (besides $\boldsymbol{\tau}_e^{(r)}$ itself). For example, if $\boldsymbol{\tau}_e^{(r)}$ is parallel to an edge e' of $F_e^{(r)}$ different from e, and is oriented from e towards the opposite vertex, then

$$\frac{\partial(\mathbf{n}_e^{(r)}\cdot\boldsymbol{\psi}_{h,e})}{\partial\tau_e^{(r)}} = -\frac{3}{2}\frac{d_e^{(r)}}{|e'|}.$$

Finally, once we know the degrees of freedom for the tangential and the normal components, it is straightforward to transform them into degrees of freedom for the Cartesian components of $\psi_{h,e}$ After performing this, the computation of $\psi_{h,e}$ reduces to the solution of a set of three (uncoupled) scalar problems of type (24).

Although only geometrical data related to the tetrahedrization are required to determine the boundary degrees of freedom for $\psi_{h,e}$, clearly enough it is too costly to compute this field for every $e \in \mathbf{E}_h$ in order to apply a discrete version of problem (23) which gives an approximation λ_h of λ. This is why we have adopted a different strategy, to be described in the next section. However, before entering into it, let us introduce the definition of the space Λ_h in which we search for λ_h.

First of all, to every $e \in \mathbf{E}_h$ we associate a spatial quadrilateral Q_e whose vertices are the extremities of e, S_e and S'_e, and the barycentres $G_e^{(r)}$, $r = 1, 2$, as illustrated in Figure 3. By definition, Λ_h is the space of functions defined on Γ_h, the boundary of Ω_h (or equivalently $\cup_{e \in \mathbf{E}_h} Q_e$), whose restriction to each Q_e is constant. Now, letting $M_h = \text{card } \mathbf{E}_h$, we have dim $\Lambda_h = M_h$ and, if we actually number the edges of $\mathbf{E}_h$ as $e_1, e_2, \ldots, e_{M_h}$, we may write

$$\lambda_h = \sum_{m=1}^{M_h} \lambda_{h,m} \chi_m, \tag{28}$$

where χ_m is the characteristic function of Q_{e_m}.

5. COMPUTATIONAL SCHEME

In principle, the so-defined discrete version of the uncoupling technique leads to an appropriate numerical solution of the equations for the vector potential. In practice, however, this can be very inefficient unless one avoids lengthy and useless computations. Two ingredients can be employed to achieve a particularly handy solution procedure.

First, the computation of the coefficients of the influence matrix can be extremely long and costly if it is necessary to know beforehand all the discrete analogues of the ψ_s's, as pointed out before. One can remedy this by replacing the 'test' functions $\psi_{s'}$ in (23) by fields $\mathbf{w}_{s'}$ satisfying the same boundary conditions as $\psi_{s'}$ but having a small support near Γ. In the discrete case this would mean a support consisting of the set of elements with a non-empty intersection with Γ_h. This simplified approach was introduced in Reference 6 for second-order vector problems and, in the context of the above defined tetrahedral element, it can be described as follows.

Let $\mathbf{w}_{h,e}$ be the field associated with edge $e \in \mathbf{E}_h$. By the same arguments exploited in the previous section to define the boundary degrees of $\psi_{h,e}$, we simply use again relations (26) and (27) to define respectively the mean value of $\mathbf{n}_e \cdot \mathbf{w}_{h,e}$ over e and the normal derivatives of the tangential

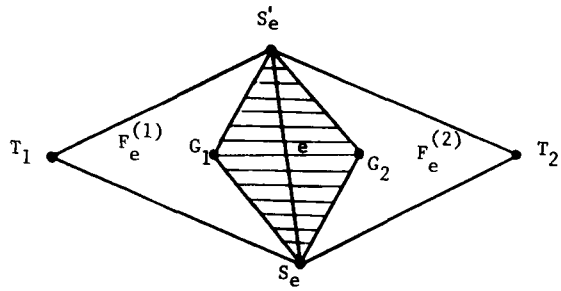

Figure 3. Quadrilateral $Q_e = S_e G_e^{(1)} S'_e G_e^{(2)}$

components of $\mathbf{w}_{h,e}$ at the barycentres of $F_e^{(1)}$ and $F_e^{(2)}$. Except for those, all the remaining degrees of freedom of $\mathbf{w}_{h,e}$ vanish by definition. Summarizing, each of the functions $\mathbf{w}_{h,e}$ is defined by only five scalars, which makes the storage requirements and computer time needed to compute them far from excessive.

Let us now turn our attention to the solution of problem (23) in its discrete version. Stated as it is, it may involve a considerable amount of computations, even for relatively coarse meshes. Here the conjugate gradient algorithm can be used in which the influence matrix is never explicitly computed, but just its product with suitable vectors to be updated along the iteration. This method, which was originally proposed in Reference 2 for the split solution of two-dimensional scalar biharmonic problems, actually leads to a very fast convergence in the determination of the solution λ_h. Both the argument and the algorithm can be better described with reference to the continuous problem.

Assume that μ is a given function of $H^{3/2}(\Gamma)$ and that the quantity

$$(A\mu)(\mathbf{s}') \equiv \int_\Gamma a(\mathbf{w}_{\mathbf{s}'}, \boldsymbol{\psi}_{\mathbf{s}})\, \mu(\mathbf{s})\, d\mathbf{s}$$

has to be computed (A being the influence matrix). We claim that

$$(A\mu)(\mathbf{s}') = a(\mathbf{w}_{\mathbf{s}'}, \boldsymbol{\psi}_\mu),$$

where $\boldsymbol{\psi}_\mu$ is the solution of the problem

$$\nu\Delta^2\boldsymbol{\psi}_\mu = \mathbf{0}, \tag{29}$$

$$\mathbf{n}\cdot\boldsymbol{\psi}_\mu|_\Gamma = \mu, \qquad \mathbf{n}\times\boldsymbol{\psi}_\mu|_\Gamma = \mathbf{0},$$

$$\nabla\cdot\boldsymbol{\psi}_\mu|_\Gamma = 0, \qquad \mathbf{n}\times\nabla\times\boldsymbol{\psi}_\mu|_\Gamma = \mathbf{0}. \tag{29a}$$

Indeed, according to an argument already employed in Section 3, we have

$$(A\mu)(\mathbf{s}') = a\left(\mathbf{w}_{\mathbf{s}'}(\cdot), \int_\Gamma \hat{\boldsymbol{\psi}}(\cdot, \mathbf{s})\, \mu(\mathbf{s})\, d\mathbf{s}\right).$$

Thus it suffices to establish that the field

$$\int_\Gamma \hat{\boldsymbol{\psi}}(\mathbf{x}, \mathbf{s})\, \mu(\mathbf{s})\, d\mathbf{s}$$

is nothing but $\boldsymbol{\psi}_\mu(\mathbf{x})$. According to the definition of $\hat{\boldsymbol{\psi}}(\mathbf{x}, \mathbf{s})$, all the homogeneous relations of (29) are trivially fulfilled. On the other hand, letting an interior point $\mathbf{x}$ tend to $\mathbf{s}'$, and denoting by $\mathbf{n}_{\mathbf{s}'}$ the unit outer normal vector with respect to Γ at $\mathbf{s}'$, we obtain from (16)

$$\lim_{\mathbf{x}\to\mathbf{s}'} \int_\Gamma \mathbf{n}_{\mathbf{s}'}\cdot\hat{\boldsymbol{\psi}}(\mathbf{x}, \mathbf{s})\, \mu(\mathbf{s})\, d\mathbf{s} = \mathbf{n}_{\mathbf{s}'}\cdot\boldsymbol{\psi}_\mu(\mathbf{s}'),$$

since this limit is

$$\langle \mathbf{n}_{\mathbf{s}'}\cdot\boldsymbol{\psi}_{\mathbf{s}'}, \mu\rangle_{3/2,\Gamma} = \langle \mathbf{n}\cdot\boldsymbol{\psi}_{\mathbf{s}'}, \mu\rangle_{3/2,\Gamma} \equiv \mu(\mathbf{s}').$$

Now the algorithm can be presented as follows: Let λ_0 be an arbitrary initial approximation of λ in $H^{3/2}(\Gamma)$. Determine $\boldsymbol{\psi}_0$ by solving the problem

$$\nu\Delta^2\boldsymbol{\psi}_0 = \nabla\times\mathbf{f},$$

$$\mathbf{n}\cdot\boldsymbol{\psi}_0|_\Gamma = 0, \qquad \mathbf{n}\times\boldsymbol{\psi}_0|_\Gamma = \mathbf{n}\times\mathbf{a},$$

$$\nabla\cdot\boldsymbol{\psi}_0|_\Gamma = 0, \qquad \mathbf{n}\times\nabla\times\boldsymbol{\psi}_0|_\Gamma = \mathbf{n}\times\mathbf{b}.$$

Then compute the residual ρ_0 given by

$$\rho_0 = \rho_0(\mathbf{s}') \leftarrow a(\mathbf{w}_{\mathbf{s}'}, \boldsymbol{\psi}_0) - \nu^{-1} \int_\Omega \mathbf{w}_{\mathbf{s}'} \cdot \nabla \times \mathbf{f}$$

and set

$$\mu_0 \leftarrow \rho_0.$$

Next, for $k = 1, 2, 3, \ldots$, compute $\boldsymbol{\psi}_k$ as the solution of the problem

$$\nu \Delta^2 \boldsymbol{\psi}_k = \mathbf{0},$$

$$\mathbf{n} \cdot \boldsymbol{\psi}_k|_\Gamma = \mu_{k-1}, \qquad \mathbf{n} \times \boldsymbol{\psi}_k|_\Gamma = \mathbf{0},$$

$$\nabla \cdot \boldsymbol{\psi}_k|_\Gamma = 0, \qquad \mathbf{n} \times \nabla \times \boldsymbol{\psi}_k|_\Gamma = \mathbf{0}$$

and set

$$(A\mu_{k-1})(\mathbf{s}') \leftarrow a(\mathbf{w}_{\mathbf{s}'}, \boldsymbol{\psi}_k).$$

Evaluate finally the quantities

$$r_k \leftarrow (\mu_{k-1}, \rho_{k-1})/(A\mu_{k-1}, \mu_{k-1}),$$

$$\lambda_k \leftarrow \lambda_{k-1} - r_k \mu_{k-1},$$

$$\rho_k \leftarrow \rho_{k-1} - r_k A \mu_{k-1},$$

$$s_k \leftarrow (\rho_k, \rho_k)/(\rho_{k-1}, \rho_{k-1}),$$

$$\mu_k \leftarrow \rho_k + s_k \mu_k$$

until $\| \lambda_k - \lambda_{k-1} \| < \varepsilon$, in which case we set $\lambda \leftarrow \lambda_k$. Here ε is a small tolerance, $\| \mu \| = (\mu, \mu)^{1/2}$ and the inner product $(.\,,.)$ is given by

$$(\mu, \rho) = \int_\Gamma \mu(\mathbf{s})\, \rho(\mathbf{s})\, \mathrm{d}\mathbf{s}.$$

Going back to the discrete case, we compute a sequence $\{\lambda_{h,k}\} \subset \Lambda_h$ of approximations of λ_h, together with $\mu_{h,k}$ and $\rho_{h,k}$ in Λ_h as well, for $k = 0, 1, 2, \ldots$, by performing the following modifications in the above algorithm, besides the obvious ones.

First, the bilinear form a is replaced by its discrete version a_h defined by

$$a_h(\boldsymbol{\psi}_h, \boldsymbol{\phi}_h) = \sum_{T \in \mathbf{T}_h} \left[\int_T \nabla \times \nabla \times \boldsymbol{\psi}_h \cdot \nabla \times \nabla \times \boldsymbol{\phi}_h + \int_T \nabla(\nabla \cdot \boldsymbol{\psi}_h) \cdot \nabla(\nabla \cdot \boldsymbol{\phi}_h) \right].$$

Then $\boldsymbol{\psi}_{h,k} \in [V_h]^3$ is computed instead of $\boldsymbol{\psi}_k$ by solving discrete problems of the type (24), in which the boundary data are deduced from $\mu_{h,k}$, basically like in the case of $\boldsymbol{\psi}_{h,e}$ described in Section 4. Notice, however, that now all the boundary edge and face degrees of freedom must be computed. The calculations are based again on the fact that any tangential derivative of the normal component of $\boldsymbol{\psi}_{h,k}$ at the barycentre of a face of $\mathbf{F}_h$ is a given linear combination of the three edge degrees of freedom associated with this face, which can be deduced directly from $\mu_{h,k}$. We skip the details for the sake of conciseness.

Finally, since we work with $\mathbf{w}_{h,e}$, $e \in \mathbf{E}_h$, instead of $\mathbf{w}_\mathbf{s}$, $\mathbf{s} \in \Gamma$, the discrete analogue $A_h \mu_h$ of $A\mu$ is first defined edge by edge and then extended to the whole boundary Γ_h as a function belonging to Λ_h. Of course, once we have λ_h, it suffices to create out of it, and in the same way as for $\boldsymbol{\psi}_{h,k}$, the boundary data for problem (24). The solution of the latter yields $\boldsymbol{\psi}_h$, the approximation of the vector potential $\boldsymbol{\psi}$.

Notice that the solution of problems of the type (24) accounts for the bulk of the total computational effort required to obtain ψ_h. However, since the very same scalar solver is employed in the whole process, there is only one matrix to be stored and factorized. Actually, the numerical results given in Reference 4 show a very good performance of such an algorithm in the sense that fast convergence is achieved at a rather low cost for three-dimensional problems.

6. CONCLUDING REMARKS

Another finite element discretization based on tricubic Hermite polynomials in parallelepipeds is currently being implemented for the solution of the problem under study. Although its application is restricted to domains which can be subdivided into rectangular portions, it should generate more accurate results since it is a conforming second-order element. A comparative numerical study with the non-conforming quadratic element considered in this paper will be reported in due course. It is also our purpose to address in the near future the question of how the numerical technique adopted in this work can be extended to the important and delicate case of non-simply connected domains. As a final comment, we add that the application of the proposed techniques to the Navier–Stokes equations is possible. However, in this case the system remains coupled owing to the convective terms. A study is currently being carried out to deal with such a difficulty by means of suitable iterative schemes.

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