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**Moving Finite Elements for the Stefan problem in
two dimensions**

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Equazioni a derivate parziali. — *Moving Finite Elements for the Stefan problem in two dimensions.* Nota (*) di ROGER ALEXANDER (**), PAOLO MANSELLI (***) e KEITH MILLER (****), presentata dal Socio G. SANSONE.

RIASSUNTO. — La presente è una Nota introduttiva sulla estensione del metodo degli Elementi Finiti Mobili a problemi con due dimensioni spaziali. Tale metodo numerico è stato sviluppato specificamente per trattare equazioni a derivate parziali non lineari le cui soluzioni sviluppano automaticamente onde d'urto. Nel presente lavoro tale metodo è applicato al problema di Stefan in due dimensioni spaziali.

I. INTRODUCTION

In this Note we sketch the first extension of the Moving Finite Element method to problems in two space dimensions, with the Stefan problem for a melting ice front as our trial example. The MFE method (applied previously with great success to many 1-dimensional parabolic and hyperbolic problems) was developed specifically to handle the many important strongly nonlinear partial differential equations whose solutions automatically develop "shocks" "near shocks", or other critical moving regions with steep gradients. These moving node methods were introduced by K. Miller and R. Miller in [5], with Burger's equation in 1-d as the trial example, and further developed and improved by K. Miller in [6], with a variety of hyperbolic and parabolic equations in 1-d (including the Stefan problem) as the trial examples. Such methods are presently under development for rather general *systems* of PDE's in 1-d including the equations of gasdynamics and combustion.

In 2-d our finite element space consists of the piecewise linear functions on a triangular mesh with moveable nodes (because of the great complexity of an MFE code we have not wanted to deal with the obvious extensions to higher order finite element spaces). The 2-d method is far more complex,

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both in theory and in computational organization, than the 1-d method, but our preliminary computational experience is that it works quite well. The nodes do automatically concentrate in the shocklike regions as needed and move with the shocks. The parameters do settle down to become fairly smooth functions of t and our implicit stiff ODE solver then allows large time steps Δt as desired.

Our trial partial differential equation is the nonlinear equation for the Stefan problem in (slightly "smeared out") enthalpy form:

$$(1) \quad v_t = L(v) \equiv (\varphi(v))_{xx} + (\varphi(v))_{yy}.$$

Here $v(x, y, t)$ denotes the enthalpy in the medium and $\varphi(v)$ the corresponding temperature. Ideally, we should have the limiting case of $\varphi'(v) = 0$ in the "mush" region ($-1 < v < 1$) and $\varphi'(v) = 1$ in the water region ($v > 1$) or in the ice region ($v < -1$); however, as is usual in theoretical studies and in computational practice we smooth out the $\varphi(v)$ curve somewhat, such that has smooth corners and that $\varphi'(v)$ remains somewhat positive ($\geq \delta > 0$) even in the mush region. This serves to smear out the infinitely thin -1 to $+1$ shock in v to a nonzero $o(\delta)$ thickness.

The numerical difficulty with standard finite difference or finite element methods applied to enthalpy form (1), see Meyer [3] for example, is that δ must often be set sufficiently high to smear the shock over several mesh widths in order to ensure decent numerical behaviour. But, since too large a δ can significantly change the global behaviour of the solution, this method will often require an extremely high nodal resolution. Bonnerot and Jamet [2] have introduced certain finite element methods with moving nodes for the Stefan problem. These methods require that the ice-water interface be essentially the graph of a function $y = y(x)$; the nodes on the interface are allowed to move only in vertical direction in order to satisfy a Stefan interface condition, and the other nodes follow along proportionately.

Our method, on the other hand, is more general and flexible; it allows the solution to seek out a general interface; the ice region can even annihilate itself, melt in two, and otherwise change topological type. We should point out that we could rather easily build into our method an absolute -1 to $+1$ enthalpy shock across certain prespecified triangle edges and such a method, closer in spirit to the Bonnerot and Jamet method, would probably be more efficient than our present method (so long as the ice region does not try to change topological type). To dwell on such a highly particular scheme for the Stefan problem, however, would miss the point of great generality and topological flexibility of our MFE methods and their promise for a wide variety of important and difficult equations.

2. OUTLINE OF THE METHOD

For simplicity we restrict ourselves to a rectangular spatial region Ω , with Dirichlet initial and boundary conditions. Our approximant u to the true solution v is a continuous piecewise linear function on a hexagonally connected triangulation of Ω , with both the amplitude $a_j(t)$ and the position $(x_j(t), y_j(t))$ at its j -th interior node being variable and unknown, $j = 1 \dots N$. These three values at the boundary nodes are given and (again, merely for simplicity) fixed. Since the initial function u_0 and the boundary function g will have to be well approximated by piecewise linear functions on Ω and $\partial\Omega$, we assume that they are already of that form. We derive ordinary differential equations for $\{\dot{a}_j, \dot{x}_j, \dot{y}_j\}$ in terms of $\{a_j, x_j, y_j\}$ by requiring that \dot{u} (which depends linearly on the $\{\dot{a}_j, \dot{x}_j, \dot{y}_j\}$) be that element which (formally) minimizes the $L^2(\Omega)$ norm $\|\dot{u} - L(u)\|^2$.

There are difficulties with degeneracies of the parametrization, but these are handled by regularization techniques involving slight "intratriangular viscosities and spring forces" on the triangles of the grid. Thus, we instead choose $\{\dot{a}_j, \dot{x}_j, \dot{y}_j\}$ so as to (formally) minimize:

$$(2) \quad \psi = \|\dot{u} - L(u)\|^2 + \sum (\varepsilon(d_k) - f(d_k))^2$$

where the sum is over all possible interior heights d_k of the triangles of the grid, $\varepsilon(d)$ is a small "intratriangular viscosity function" and $f(d)$ is a small "intratriangular spring function".

The canonical equations for (formally) minimizing ψ in (2) can be obtained by taking the partials of ψ with respect to the unknowns $\{\dot{a}_j, \dot{x}_j, \dot{y}_j\}$ and setting these equal zero. Since the canonical equations for minimizing the sum of the two terms in (2) is just the sum of the canonical equations for the two terms separately, for sake of simplicity let us just discuss the canonical equations for the first term $\|\dot{u} - L(u)\|^2$ in (2). The equations for the second term will be analogous and much simpler. Notice that by the chain rule

$$(3) \quad \dot{u} = \sum_{j=1}^N \dot{a}_j \frac{\partial u}{\partial a_j} + \dot{x}_j \frac{\partial u}{\partial x_j} + \dot{y}_j \frac{\partial u}{\partial y_j} \equiv \sum_{j=1}^N \dot{a}_j \alpha^j + \dot{x}_j \beta^j + \dot{y}_j \gamma^j.$$

Here a few diagrams would be helpful to visualize the form of the functions $\alpha^j = \partial u / \partial a_j$, $\beta^j = \partial u / \partial x_j$, $\gamma^j = \partial u / \partial y_j$. Taking tiny increments in a_j , or x_j , or y_j , one sees that all three functions are piecewise linear functions having their support in the hexagon of six triangles surrounding the j -th node. Here α^j is continuous and takes on the value 1 at the center of the hexagon and 0 at the other nodes. The function β^j on the other hand is discontinuous at the center and on the inner edges of the hexagon; it is $\equiv 0$ on the hexagonal boundary and takes on the six different values of $-u_x$ (the constant value of $\partial u / \partial x$ on each triangle) at the central vertices of the six triangles; γ^j is similar but with the six values of $-u_y$ instead.

The desired canonical equations (ignoring the regularization terms in (2)) then become that $u_t - L(u) = u_t - \Delta\varphi$ must be orthogonal to all the basis functions $\alpha^i, \beta^i, \gamma^i$; that is:

$$(4) \quad \begin{aligned} \sum_j (\alpha^j, \alpha^i) \dot{a}_j + (\beta^j, \alpha^i) \dot{x}_j + (\gamma^j, \alpha^i) \dot{y}_j &= (L(u), \alpha^i) \\ \sum_j (\alpha^j, \beta^i) \dot{a}_j + (\beta^j, \beta^i) \dot{x}_j + (\gamma^j, \beta^i) \dot{y}_j &= (L(u), \beta^i) \\ \sum_j (\alpha^j, \gamma^i) \dot{a}_j + (\beta^j, \gamma^i) \dot{x}_j + (\gamma^j, \gamma^i) \dot{y}_j &= (L(u), \gamma^i) \end{aligned}$$

for all $i = 1, \dots, N$.

In this way we obtain a system of $3N$ ordinary differential equations of the form:

$$(5) \quad C(z) \dot{z} = g(z)$$

where $z(t)$ is the vector of unknown parameters and the "mass matrix" $C(z)$ is symmetric and positive definite.

3. NUMERICAL SOLUTION OF THE ODE'S

This quite stiff system has been solved by using the high order accurate DIRK (diagonally implicit Runge-Kutta) package of the first author (see Alexander [1] and Miller [4]). This package has an automatic stepsize changer (depending on an estimation of the local truncation error) which allows the time step Δt to increase to large values when the $a_j(t), x_j(t), y_j(t)$ settle down to become very smooth functions of t .

DIRK, like most implicit ODE solvers, can be considered to be a succession of basic backward Cauchy-Euler (BCE) steps interspersed with interpolations and extrapolations. A single BCE step involves replacing \dot{z} in (5) by the backward difference $(z - \tilde{z})/\Delta t$, where \tilde{z} is a known past value and z is the unknown future value. One is thus left with the implicit equations

$$(6) \quad R(z) \equiv C(z) (z - \tilde{z})/\Delta t - g(z) = 0.$$

The formulation and organization of the computer code to solve these implicit equations is quite a massive and interesting task in itself; the inner products $(\Delta\varphi, \beta^i)$, etc. can be evaluated exactly and the contributions to the residual vector $R(z)$ can be built up triangle by triangle and edge by edge. It is not possible however, to go into the further details in this short note.

Our FORTRAN program, developed and run on the CDC 7600 of Lawrence Berkeley Labs, has been tried out on several small to moderate sized test examples. The program could use some major (and fairly difficult to program) improvements for the sake of greater computational efficiency, but the results so far have still been quite gratifying.

As mentioned in the introduction, the nodes do move with the shock as needed and the Δt does increase to decently large values. Moreover, the method does allow the ice region to change topological type; in one trial run the ice (initially in a dumbbell shaped form) quite successfully and routinely melts into two pieces.

The present note is a short and schematic presentation of the method and preview of the results obtained; for fuller details on the method, with descriptions and diagrams of the computer runs, we refer to a forthcoming paper in the writeup stage.

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