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A NUMERICAL APPROACH TO THE DISCRETE MORSE SEMIFLOW

HIDETOSHI YOSHIUCHI[1] (吉内 栄利)   SEIRO OMATA[2] (小俣 正朗)

0. Abstract

In this paper, we treat a numerical analysis of discrete Morse semiflows for energy minimizing harmonic mapping. Discrete Morse semiflows were introduced by Rektorys and Kikuchi for approximating solution of heat equations associated to variational problems. Inspired by Kikuchi's results, several authors use this method for constructing weak solutions of parabolic equations. We apply this flow to the numerical analysis and develop energy minimizing algorithm for solving approximate heat equation.

1. Introduction

In this paper, a numerical analysis of discrete Morse semiflows for harmonic mapping from $\mathbf{B}^3$ to S^2 is studied. This is considered to be the approximation of the heat flow of the following elliptic problem: Minimize the functional;

$$\mathcal{I}(u) = \int_{\mathbf{B}^3} |\nabla u|^2 dx, \quad u|_{\partial \mathbf{B}^3} = \varphi \text{ in } H^1_\varphi(\mathbf{B}^3; S^2).$$

Some authors have studied this problem from a numerical point of view. (See [Al] for example.)

Here, we present an new algorithm which use the discrete Morse semiflow for solving heat equation. For this purpose, we introduced the following time-semidiscretized functional;

$$J^h_m(u) = \int_{\mathbf{B}^3} \frac{|u - u_{m-1}|^2}{h} d\mathcal{L}^n + \mathcal{I}(u), \qquad (m = 1, 2, \cdots). \tag{1.1}$$

The procedure of determining sequence is as the following: Let u_0 be a given initial data satisfying

$$u_0 \in \mathcal{K}, \quad \text{and} \quad \mathcal{I}(u_0) < \infty,$$

where $\mathcal{K}$ is an admissible function space of the original functional $\mathcal{I}$ (In this case $\mathcal{K} = H^1_\varphi(\mathbf{B}^3; S^2)$). Taking u_0 as u_{m-1} ($m = 1$ is assumed) in $\mathcal{K}$, we define a minimizer u_1 of J_1. Inductively we define u_m by the minimizer of J_m in $\mathcal{K}$. We will call $\{u_m\}$ the **discrete Morse semiflow**.

Since the minimizers $\{u_m\}$ depend on the positive constant h, we should write $\{u^h_m\}$. But sometimes we use the notation $\{u_m\}$ when no confusions may occur.

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(1) ULVAC corporation: Hagisono 2500, Chigasaki, 253 Japan.
(2) Department of Mathematics, Faculty of Science, Kanazawa University: Kakuma-machi, Kanazawa, 920-11 Japan.
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Using this approach, Kikuchi constructed solutions of parabolic equations associated to a variational functional of harmonic map type in [K]. Nagasawa and Omata have studied the asymptotic behavior of this flow on some free boundary problems. (See [NO1] and [NO2].) On the other hand, Bethuel, Coron, Ghidaglia and Soyeur ([BCGS]) also showed the existence of the Morse semiflow associated to relaxed energies for harmonic mapping by this procedure.

2. Main property of the discrete Morse semiflow

Apart from the harmonic mapping, we here mention the basic property of the discrete Morse semiflow. Among almost all quadratic functional $\mathcal{F}(u)$, we can determine the discrete Morse semiflow is the same way as in section 1 and they have the following property:

$$J_m^h(u_m^h) \equiv \int_\Omega \frac{|u_m^h - u_{m-1}^h|^2}{h} dx + \mathcal{F}(u_m^h) \leq J_m^h(u_{m-1}^h) \equiv \mathcal{F}(u_{m-1}^h),$$

therefore

$$\int_\Omega \frac{|u_m^h - u_{m-1}^h|^2}{h} \leq \mathcal{F}(u_{m-1}^h) - \mathcal{F}(u_m^h). \tag{2.1}$$

Summing up from $m = 1$ to N, the following estimate holds:

$$\mathcal{F}(u_N^h) + \sum_{m=1}^{N} \int_\Omega \frac{|u_m^h - u_{m-1}^h|^2}{h} dx \leq \mathcal{F}(u_0). \tag{2.2}$$

This is a basic and important estimate of this flow. Many properties is to be obtained from (2.2).

We can regard such sequences of minimizers as approximate solutions of the heat equation. For this, we will introduce following two functions.

DEFINITION 2.1. *We define functions $\bar{u}^h$ and u^h on $\Omega \times (0, \infty)$ by*

$$\bar{u}^h(x,t) = u_m^h(x)$$
$$u^h(x,t) = \frac{t - (m-1)h}{h} u_m^h(x) + \frac{mh - t}{h} u_{m-1}^h(x)$$

for $(x,t) \in \Omega \times ((m-1)h, mh]$.

It is easy to see that the functions above satisfy the following relations:

$$\frac{\partial u^h(x,t)}{\partial t} = \delta\mathcal{F}\bar{u}^h(x,t) \qquad \text{in some weak sense in} \qquad \Omega \times \bigcup_{m=2}^{\infty}((m-1)h, mh)$$
$$\bar{u}^h(x,t) = u^h(x,t) = u_0(x) \qquad \text{on} \qquad \partial\Omega$$
$$u^h(x,0) = u_0(x) \qquad \text{in} \qquad \Omega.$$

Here, we investigate the convergence theory when h tends to zero. We can easily obtain the following results.

THEOREM 2.3. *If $\mathcal{F}$ is corecive, then the following norms are uniformly bounded with respect to h.*

$$\|\frac{\partial u^h}{\partial t}\|_{L^2((0,\infty)\times\Omega)}, \quad \|\nabla \bar{u}^h\|_{L^\infty((0,\infty);L^2(\Omega))}, \quad \|\nabla u^h\|_{L^\infty((0,\infty);L^2(\Omega))},$$
$$\|u^h\|_{L^\infty((0,\infty);L^2(\Omega))}, \quad \|\bar{u}^h\|_{L^\infty((0,\infty);L^2(\Omega))}, \quad \|u^h\|_{W^{1,2}((0,T)\times\Omega)} \quad (\textit{ for all} \quad T>0).$$

THEOREM 2.4. *There exists a subsequence, such that*

$$\bar{u}^h \to u \quad \textit{weakly star in} \quad L^\infty((0,\infty);L^2(\Omega)) \tag{2.3}$$
$$u^h \to u \quad \textit{weakly in} \quad W^{1,2}((0,T)\times\Omega) \tag{2.4}$$
$$u^h \to u \quad \textit{strongly in} \quad L^2((0,T)\times\Omega) \tag{2.5}$$
$$\bar{u}^h \to u \quad \textit{strongly in} \quad L^2((0,T)\times\Omega). \tag{2.6}$$

These properties follow from the basic estimate (2.2) and the following theorem.

THEOREM 2.5. *The function $\bar{u}^h$ and u^h converge to the same function u in the following sense for any T:*

$$\begin{aligned} \bar{u}^h &\to u \quad \textit{weakly in} \quad L^2(\Omega\times(0,T)) \\ u^h &\to u \quad \textit{weakly in} \quad H^1(\Omega\times(0,T)) \\ &\qquad \textit{and strongly in} \quad L^2(\Omega\times(0,T)). \end{aligned}$$

Proof. From (2.2), we have

$$\int_\Omega |\nabla \bar{u}^h(x,Nh)|^2 dx + \int_0^{Nh}\int_\Omega \left|\frac{\partial u^h}{\partial t}(x,t)\right|^2 dx$$
$$\leq \mathcal{F}(u_0).$$

It implies that $\{\bar{u}^h\}_{h>0}$ and $\{u^h\}_{h>0}$ are bounded sets in $L^2(\Omega\times(0,T))$ and $H^1(\Omega\times(0,T))$ respectively for any $T>0$. Therefore we can extract a subsequence $\{h_j\}$ such that $h_j \downarrow 0$ and

$$\begin{aligned} \bar{u}^{h_j} &\to u \quad \text{weakly in} \quad L^2(\Omega\times(0,T)) \\ u^{h_j} &\to v \quad \text{weakly in} \quad H^1(\Omega\times(0,T)) \\ &\qquad \text{and strongly in} \quad L^2(\Omega\times(0,T)) \end{aligned}$$

as $j\to\infty$.

It follows from $|u^h - \bar{u}^h| \leq |\frac{\partial u^h}{\partial t}|$ that

$$\int_0^T\int_\Omega |u^h - \bar{u}^h|^2 dxdt \leq h^2 \int_0^\infty \int_\Omega \left|\frac{\partial u^h}{\partial t}\right|^2 dxdt$$
$$\leq h^2\mathcal{F}(u_0) \to 0 \quad \text{as} \quad h\downarrow 0,$$

which shows $u=v$. ∎

3. Recent results on the Harmonic Mapping into Sphere

Bethuel, Coron, Ghidaglia and Soyeur constructed weak heat flows related to the Harmonic mapping from $\mathbf{B}^3$ to S^2 by using this flow. We here only mention their result related to this paper.

THEOREM 3.1. *Let u_0 and γ belong to $H^1(\mathbf{B}^3; S^2)$ with $u_0 = \gamma$ on $\partial\mathbf{B}^3$. There exists a weak solution to*

$$\frac{\partial u}{\partial t} - \Delta u = u|\nabla u|^2 \tag{3.1}$$

$$u(x,t) = \gamma(x), \quad t > 0, \quad x \in \partial\mathbf{B}^3 \tag{3.2}$$

$$u(x,0) = u_0(x), \quad x \in \mathbf{B}^3. \tag{3.3}$$

4. Numerical analysis

We mention here a minimizing algorithm used in this paper. The minimizing algorithm means some procedure that determine sequence of comparison function which will converge to the minimizer. Our method is based on the simplex search method which is one of the finite element method. The scheme of the simplex search method is as follows: (1) Discretize the domain into the suitable elements which is called finite element. (We will assume that the domain is divided into M elements with N nodes.) (2) Approximate the comparison function by using the piecewise linear function which is coincide with original comparison function on nodal points. By this approximation, we can regard the elements of R^N as the approximate comparison function. (3) Generate a simplex in R^N. The simplex consist of $N+1$ vertices. (4) Calculate the value of the functional at each vertex of the simplex, and find the maximizer(the vertex where the value of the functional is the largest). Then, move the maximizing point to the opposite side of hyperplane which is spanned by another vertices. By this procedure, we can make a new simplex. (5) Repeat this step up to satisfy the given terminate conditions.

Throughout these procedures, we expect to find an approximate minimizer.

We proceed discretization along to this algorithm using finite elements. Firstly, split $\mathbf{B}^3$ into M small finite elements(tetrahedron) with N nodes. In order to use the simplex search method, we choose values of all nodal points. Secondly, approximate a comparison function u by the linear function,

$$\begin{aligned} \tilde{u} &= \{\tilde{u}_1, \tilde{u}_2, \tilde{u}_3\} \\ \tilde{u}_i &= A_i x_1 + B_i x_2 + C_i x_3 + D_i, \end{aligned}$$

in an finite element, which coincide with the given data on the nodal point. (A_i, B_i, C_i, and D_i are uniquely determined by the value at each nodal point.)

Thirdly, calculate the value of the functional for the approximate function. For calculation, we introduce the following penalized variational problem: Minimize

$$\tilde{J}^h_m(u) = \int_{\mathbf{B}^3} \left(\frac{|u - u_{m-1}|^2}{h} + |\nabla u|^2 + \frac{1}{\varepsilon}(|u|^2 - 1)^2 \right) dx, \tag{4.1}$$

in $u \in H^1_\varphi(\mathbf{B}^3; \mathbf{R}^3)$.

We use the following discretization for $\tilde{J}^h_m(u)$:

$$\int_{\mathbf{B}^3} \frac{|u-u_{m-1}|^2}{h} dx = \frac{1}{h}\sum_{k=1}^{M}\left(\sum_{i=1}^{3}\left(\sum_{l=1}^{16}(u^{sub}_{i,k,l})^2 \times (vol_k/16)\right)\right) \tag{4.2}$$

$$\begin{aligned}\int_{\mathbf{B}^3} |\nabla u|^2 dx &= \sum_{k=1}^{M}\left(\sum_{i,j=1}^{3}\left(\frac{\partial \tilde{u}_i}{\partial x_j}\right)^2 \times vol_k\right)\\ &= \sum_{k=1}^{M}\left(\sum_{i=1}^{3}(A^2_{i,k}+B^2_{i,k}+C^2_{i,k}) \times vol_k\right)\end{aligned} \tag{4.3}$$

$$\int_{\mathbf{B}^3} \frac{1}{\varepsilon}(|u|^2-1)^2 dx = \sum_{j=1}^{N}\sum_{i=1}^{3}\frac{1}{\varepsilon}\left((u_{i,j})^2-1\right)^2 \tag{4.4}$$

where $u_{i,j}$ and $u_{i,j,m-1}$ denote the value of the function $u_i(x)$ and $u_{i,m-1}(x)$ at the jth node respectively, vol_k denotes the volume of the kth element and $A_{i,k}, B_{i,k}, C_{i,k}$ denote the coefficients of the approximated function $\tilde{u}_i(x)$ on kth element. For the term (4.2), we divide an element into 16 subelements and assume that the function $|u-u_{m-1}|^2$ is linear on the each subelement. $u^{sub}_{i,k,l}$ denotes the the value of the approximated $|u_i - u_{i,m-1}|^2 (i=1,2,3)$ on the lth subelement in the kth element.

5. Result

We calculate, here, both linear(without term 4.4) and nonlinear cases. In the linear case, we adopt the following conditions.

(1) Initial data:

$$u_0(x) = f_z^{-1}(x) \qquad \text{where} \qquad f_z(x) = (1-|x|)z + x, \qquad \exists z \in \mathbf{B}^3.$$

(2) Boundary condition:

$$u_m(x)|_{\partial \mathbf{B}^3} = i.d. \quad (m = 1, 2, \cdots)$$

(3) Parameters:

$$(\varepsilon = +\infty), \qquad h = 0.1 \qquad z = (0,\, 0,\, 0.9).$$

Figure 1 and 2 denotes u_0 and u_1 respectively in the linear case. In figures, arrows denotes vector field inside of $\mathbf{B}^3$. (Boundary data are omitted.)

In the nonlinear case, we calculate this under the following conditions.

(1) Initial data:

$$u_0(x) = p(f_z^{-1}(x)) \qquad \text{where} \qquad f_z(x) = (1-|x|)z + x, \qquad \exists z \in \mathbf{B}^3 \quad p(x) = \frac{x}{|x|}.$$

(2) Boundary condition:

$$u_m(x)|_{\partial \mathbf{B}^3} = i.d. \quad (m = 1, 2, \cdots)$$

(3) Parameters:

$$\varepsilon = 0.01, \qquad h = 0.1 \qquad z = (0,\, 0,\, 0.9).$$

Figure 3, 4 and 5 denotes u_0, u_1 and u_2 respectively. Also, arrows denotes vector field.

Because h relatively is large, the singular points moves very fast in the first time step. It is very natural to consider that the motion of the singular points depends on the parameter h and ε. Thus, we should calculate carefully changing these parameters. But unfortunately, we do not have enough computer power. Up to now, we only calculate the case when $h = 0.1$ and $\varepsilon = 0.01$. We are now proceeding this research in this point of view.

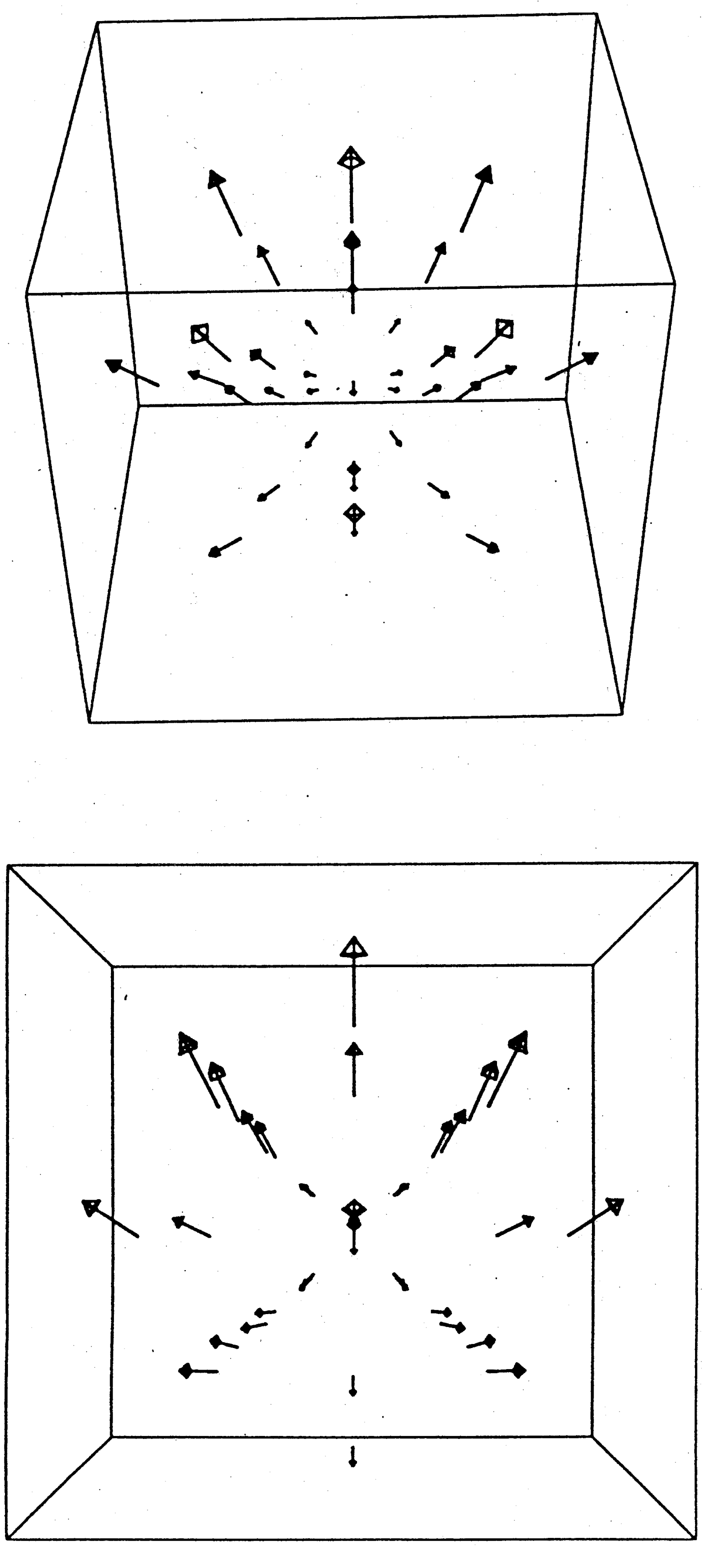


Figure 1 - Initial Data (Linear)

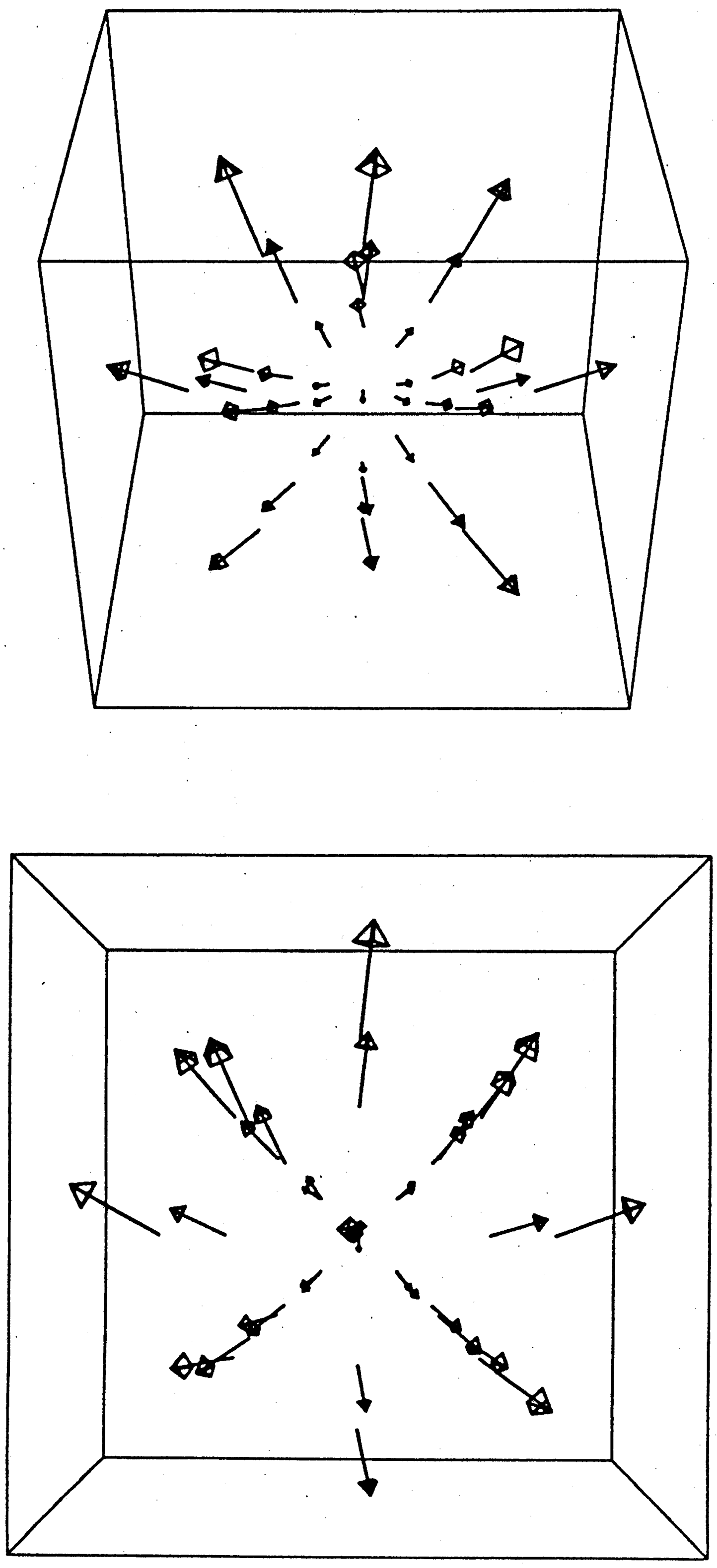
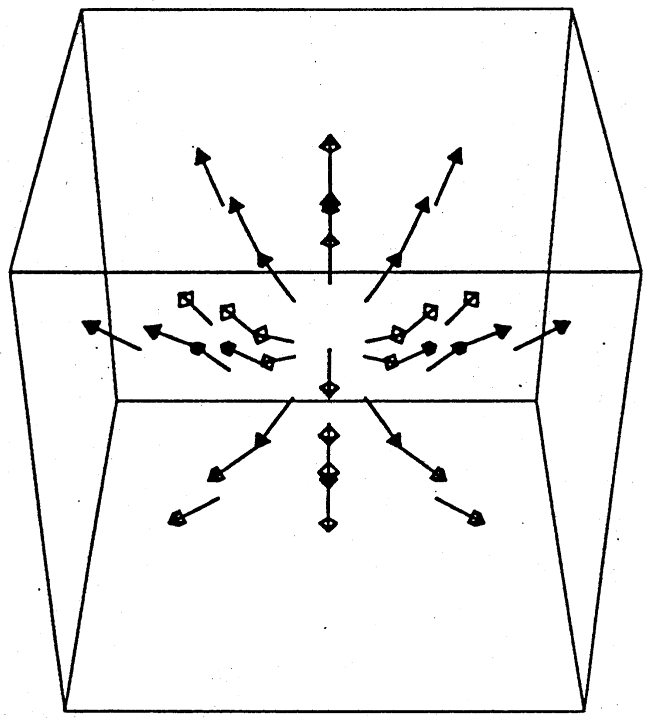


Figure 2 - u(x):m=1 (Linear)



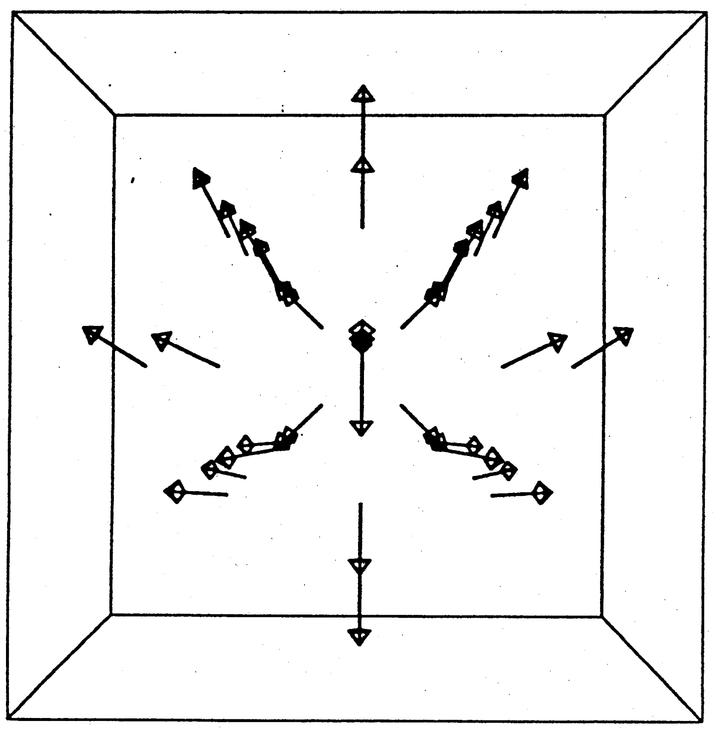


Figure 3 - Initial Data (Non-Linear)

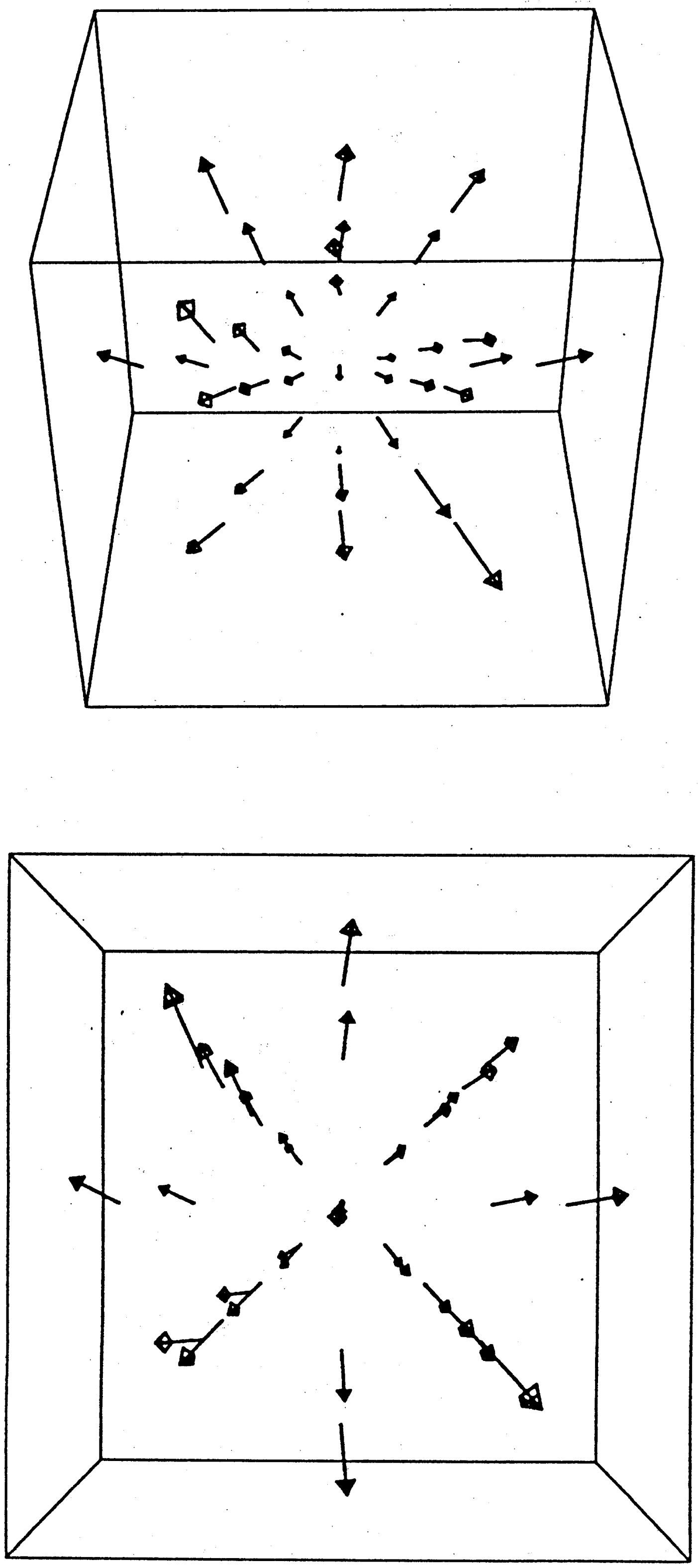


Figure 4 - u(x):m=1 (Non-Linear)

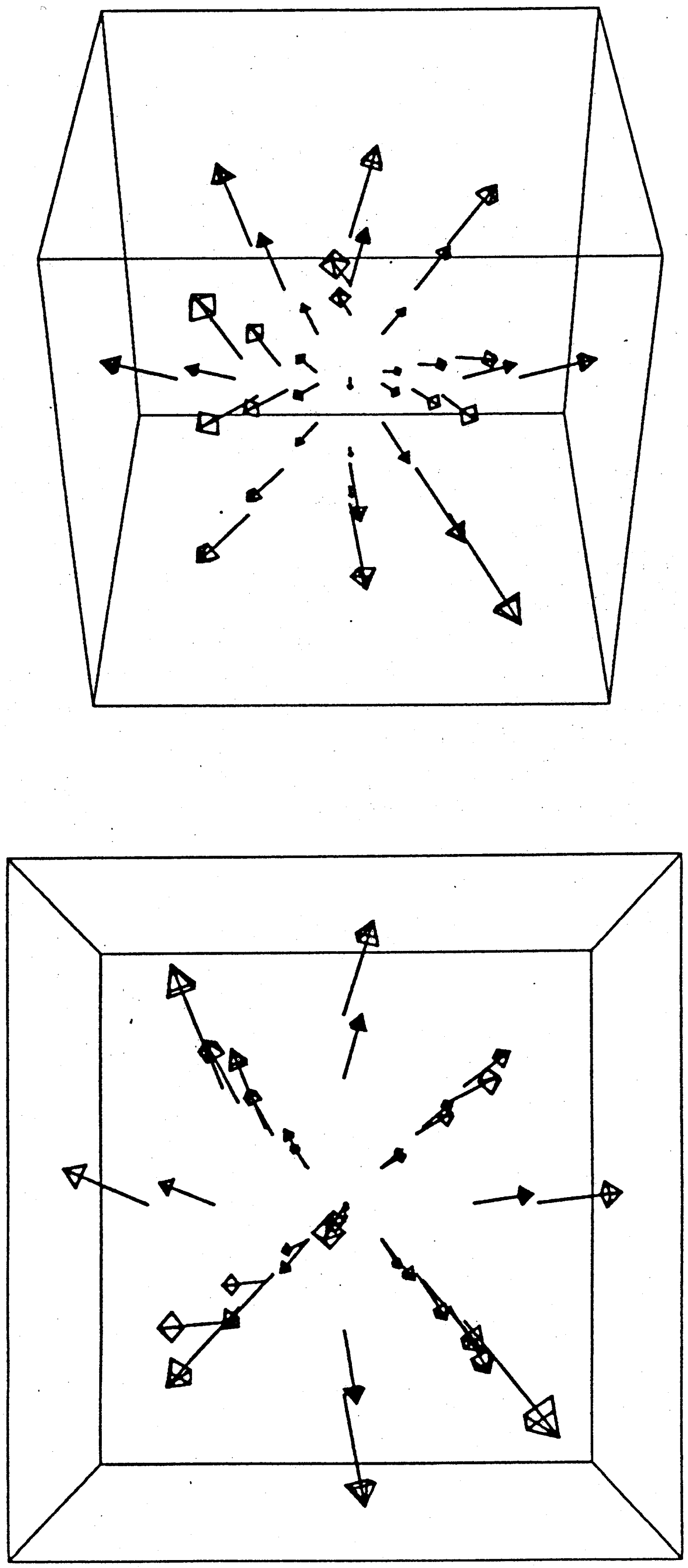


Figure 5 - u(x):m=2 (Non-Linear)

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