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Author(s)	NAKANE, KAZUAKI; OKAMURA, TOSHIHIRO; OMATA, SEIRO
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NUMERICAL ANALYSIS FOR THE DISCRETE MORSE SEMIFLOW

中根 和昭 岡村 敏弘 小保 正朗
KAZUAKI NAKANE TOSHIHIRO OKAMURA SEIRO OMATA

Department of Mathematics, Faculty of Science, Kanazawa University

1. Definition of discrete Morse semiflows

We treat numerical analysis for an approximate solution of a heat flow related to a minimizing problem of a functional (1.1) below. Our method leads to a new (general) treatment of a numerical analysis for heat flows (See [4]). Moreover, by use of a limit function of this flow, we can obtain a solution of an elliptic problem with better regularity.

Let $\Omega \subset \mathbf{R}^n$ be a bounded domain with a smooth boundary ($n \geq 1$). Consider a minimizing problem of the functional:

$$I(u) := \int_{\Omega} (|\nabla u|^2 + f(u)) dx, \quad \text{in } \mathcal{K} = W_{\varphi}^{1,2}(\Omega; \mathbf{R}^N), \quad (1.1)$$

where $N \geq 1$ and \mathcal{K} is an admissible function space whose elements are square summable up to the first (weak) derivative and satisfy boundary data, φ , in the sense of trace. Moreover f is a nonnegative function. In this paper, f will be chosen in the following:

$$f(u) := \frac{1}{\delta} (|u|^2 - 1)^2 \quad \text{Ginzburg-Landau type } (n = N = 2) \quad (1.2)$$

$$f(u) := \chi_{u>0}(x) \quad \text{Free boundary problem } (n = 2, N = 1). \quad (1.3)$$

We introduce the notion of the discrete Morse semiflow. For many types of energy functional, we can consider the following type of time semidiscretized functional. Let h be a positive number which tends to zero later. Consider the energy functionals:

$$J_m(u) = \int_{\Omega} \frac{|u - u_{m-1}|^2}{h} dx + I(u), \quad (m = 1, 2, \dots). \quad (1.4)$$

We will determine the sequence $\{u_m\}$ of functions in \mathcal{K} inductively. Firstly, for any $u_0 \in \mathcal{K}$ with $I(u_0) < \infty$, we define u_1 , as the minimizer of J_1 in \mathcal{K} . The next function $u_2 \in \mathcal{K}$ is the minimizer of J_2 in \mathcal{K} , and so on.

Since the minimizers $\{u_m\}$ depend on the positive constant h , we should write $\{u_m^h\}$ and also $J_m = J_m^h$. However we use the notation $\{u_m\}$ and J_m unless any confusions occur.

The function u_m satisfies the following Euler-Lagrange equation when f is differentiable:

$$\int_{\Omega} \left(2 \frac{u_m - u_{m-1}}{h} \phi + 2 \nabla u_m \nabla \phi + f'(u_m) \phi \right) dx = 0 \quad (1.5)$$

for any $\phi \in C_0^\infty(\Omega; \mathbf{R}^N)$. The equation (1.5) is the time-semidiscretization of the heat equation which possibly describes the Morse semiflow for $I(u)$. Hence, we call $\{u_m\}$ the **discrete Morse semiflow**.

This approach to determine the family $\{u_m\}$ by the minimality of the auxiliary functional J_m is proposed by Kikuchi in [1] and related result can be found in [2,3,4].

2. Uniqueness

In this section, we consider the uniqueness of a discrete Morse semiflow.

Theorem 2.1. *Let u and v be minimizers of (1.4). If $f''(u)$ is bounded then the second variation formula becomes positive when we choose h small enough.*

Proof. We have

$$\left. \frac{d^2}{d\varepsilon^2} J_m(u + \varepsilon\phi) \right|_{\varepsilon=0} = \int_{\Omega} \left(\left(\frac{2}{h} + f''(u) \right) \phi^2 + 2|\nabla\phi|^2 \right) dx. \quad (2.1)$$

If we choose h small enough, we can make (2.1) positive. It implies the functional J_m is unily determined. \square

Now, we shall mention for each case (1.2) and (1.3). For the case (1.2), by the choise of testing function $v = u/|u|$, we can show the minimizers are bounded. And for the case (1.3), if we choose suitable approximation function $\chi_{u>0}^\varepsilon$ (see (7.1) for definition), we can make $\chi_{u>0}^{\varepsilon''}$ is bounded. Therefore the both of the cases, the discrete Morse semiflows are uniquely determined.

Remark 2.1. In the case (1.3), by using maximam principle, we have each minimizer u_m is bounded.

By use of this theorem, it becomes very easy for us to make a good algorithm for seeking a minimizer.

3. Convergence theory for $h \rightarrow 0$

The essential estimate on this flow is based on the following property:

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

and therefore we have

$$\int_{\Omega} \frac{|u_m^h - u_{m-1}^h|^2}{h} dx \leq I(u_{m-1}^h) - I(u_m^h). \quad (3.1)$$

Summing up from $m = 1$ to M , we have the estimate:

$$I(u_M^h) + \sum_{m=1}^M \int_{\Omega} \frac{|u_m^h - u_{m-1}^h|^2}{h} dx \leq I(u_0). \quad (3.2)$$

This estimate is a basic estimate of this flow, from which many properties are obtained.

Before showing the convergence theory, firstly, we define the approximate solution of the heat equation related to (1.2).

Definition 3.1. We define functions \bar{u}^h and u^h on $\Omega \times (0, \infty)$ by

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

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

It is easy to see that the functions above satisfy the following relations in a weak sense:

$$\begin{aligned}\frac{\partial u^h(x, t)}{\partial t} &= \Delta \bar{u}^h(x, t) - \frac{1}{2} f'(\bar{u}^h) \quad \text{in } \Omega \times \bigcup_{m=2}^{\infty} ((m-1)h, mh), \\ \bar{u}^h(x, t) &= u^h(x, t) = u_0(x) \quad \text{on } \partial\Omega, \\ u^h(x, 0) &= u_0(x) \quad \text{in } \Omega.\end{aligned}$$

Here, we investigate the convergence theory when h tends to zero. By use of (3.2), we can easily obtain the following results.

Theorem 3.2. The following norms are uniformly bounded with respect to h :

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

Theorem 3.3. There exists a subsequence, such that

$$\bar{u}^h \rightarrow u \quad \text{weakly star in } L^\infty((0, \infty); L^2(\Omega)), \quad (3.3)$$

$$\nabla \bar{u}^h \rightarrow \nabla u \quad \text{weakly star in } L^\infty((0, \infty); L^2(\Omega)), \quad (3.4)$$

$$u^h \rightarrow u \quad \text{weakly in } W^{1,2}((0, T) \times \Omega), \quad (3.5)$$

$$u^h \rightarrow u \quad \text{strongly in } L^2((0, T) \times \Omega), \quad (3.6)$$

$$\bar{u}^h \rightarrow u \quad \text{strongly in } L^2((0, T) \times \Omega), \quad (3.7)$$

By use of above estimates, we have:

Theorem 3.4. Functions \bar{u}^h and u^h converge to the same function u in the following sense: For any T ,

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

Proof. From (3.2), we have the estimate

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

It implies that $\{\bar{u}^h\}_{h>0}$ and $\{u^h\}_{h>0}$ are bounded sets in $L^2(\Omega \times (0, T))$ and $W^{1,2}(\Omega \times (0, T))$ respectively for any $T > 0$. Therefore we can extract a subsequence $\{h_j\}$ such that $h_j \downarrow 0$ and $\bar{u}^{h_j} \rightharpoonup u$ weakly in $L^2(\Omega \times (0, T))$, $u^{h_j} \rightharpoonup v$ weakly in $W^{1,2}(\Omega \times (0, T))$ and strongly in $L^2(\Omega \times (0, T))$ as $j \rightarrow \infty$. It follows from $|u^h - \bar{u}^h| \leq h \left| \frac{\partial u^h}{\partial t} \right|$ that

$$\int_0^T \int_{\Omega} |u^h - \bar{u}^h|^2 dx dt \leq h^2 \int_0^{\infty} \int_{\Omega} \left| \frac{\partial u^h}{\partial t} \right|^2 dx dt \leq h^2 I(u_0) \rightarrow 0 \quad \text{as } h \downarrow 0,$$

which shows $u = v$. □

By use of Theorem 3.4, we can show that the limit function satisfies the following equation: Here, in general, we assume the following:

Assumption 3.5. *There is a constant $M > 0$ such that*

$$\|u^h\|_{L^\infty((0,T) \times \Omega)} \leq M \quad \text{and} \quad \|\bar{u}^h\|_{L^\infty((0,T) \times \Omega)} \leq M \quad (\text{for all } T > 0) \quad \text{hold.}$$

Theorem 3.6. *If f' is continuous and u^h and \bar{u}^h satisfies Assumption 3.3, then the limit function u belongs to $\mathring{V}_2((0, T) \times \Omega)$ and satisfies*

$$\int_{\Omega} u_0 \eta(x, 0) dx = \int_0^T \int_{\Omega} D_t u \eta dx dt + \int_0^T \int_{\Omega} D u D \eta dx dt + \int_0^T \int_{\Omega} f'(u) \eta dx dt \quad (3.8)$$

for all $\eta \in \mathring{W}_2^{1,1}((0, T) \times \Omega)$ with $\eta(x, T) = 0$, where $\mathring{V}_2((0, T) \times \Omega) = \{u \in L^2(Q_T), u_x \in L^2(Q_T); |u|_{Q_T} = \text{esssup}_{0 \leq t \leq T} \|u(x, t)\|_{L^2(\Omega)} + \|u_x\|_{L^2(Q_T)} < \infty\}$. We call the function u a weak solution.

Proof. Obviously, approximate solutions satisfy

$$\int_{\Omega} u_0 \eta(x, 0) dx = \int_0^T \int_{\Omega} D_t u^h \eta dx dt + \int_0^T \int_{\Omega} D \bar{u}^h D \eta dx dt + \int_0^T \int_{\Omega} f'(\bar{u}^h) \eta dx dt.$$

Thus Theorem 3.4 guarantees that approximate solutions converge to u which satisfy (3.8). □

4. Convergence theory for $m \rightarrow \infty$

In this section we investigate the asymptotic behavior of the discrete Morse semiflow $\{u_m\}$ as $m \rightarrow \infty$. From the inequality (3.2), we easily have the following:

Lemma 4.1. *We have the $L^2(\Omega)$ -decay of differences $u_m - u_{m-1}$ as $m \rightarrow \infty$, i.e., $\|u_m - u_{m-1}\|_{L^2(\Omega)} \rightarrow 0$ as $m \rightarrow \infty$.*

Now we show the existence of limit u_∞ of a subsequence.

Theorem 4.2. For any subsequence $\{u_{m_j}\} \subset \{u_m\}$, there exists a subsequence $\{u_{m_{j\nu}}\} \subset \{u_{m_j}\}$ and a function u_∞ on Ω such that

$$u_{m_{j\nu}} \rightharpoonup u_\infty \quad \text{weakly in } W^{1,2}(\Omega), \quad (4.1)$$

$$u_{m_{j\nu}} \rightarrow u_\infty \quad \text{in } L^2(\Omega), \quad (4.2)$$

as $\nu \rightarrow \infty$. Moreover, we have

$$u_\infty = u_0 \quad \text{on } \partial\Omega \quad \text{in the sense of trace.} \quad (4.3)$$

Proof. Since $\{J_m(u_m)\}$ is a non-increasing sequence, $\{u_m\}$ is weakly compact in $W^{1,2}(\Omega)$. Therefore (4.1) and (4.2) hold by use of the weak compactness argument and Rellich's theorem. The boundary condition (4.3) follows from (4.1). \square

Theorem 4.3. The limit u_∞ is a minimizer of the functional

$$J_\infty(u) = \int_\Omega \left(\frac{|u - u_\infty|^2}{h} + |\nabla u|^2 + f(u) \right) dx$$

in \mathcal{K} , hence, u_∞ satisfies

$$- \int_\Omega \left(2\nabla u_\infty \nabla \phi + f'(u_\infty) \phi \right) dx = 0 \quad \text{for any } \phi \in C_0^\infty(\Omega).$$

By use of a general theory, we can easily obtain the result, thus the proof is omitted.

5. On the numerical method

We mention here a minimizing algorithm used in this paper. Our method is based on the finite elements method. We proceed discretization into finite elements. Firstly, split Ω into Q small finite elements (triangle) with P nodes inside of Ω . Secondly, approximate a comparison function u by a piecewise linear function,

$$\begin{aligned} \tilde{u} &= \{\tilde{u}_1, \tilde{u}_2, \dots, \tilde{u}_N\} \\ \tilde{u}^i &= A_1^i x_1 + \dots + A_j^i x_j + \dots + A_n^i x_n + C_j, \end{aligned}$$

in a finite elements, which coincides with the given data at each nodal point. $\{A_j^i\}$, and C_j are uniquely determined by the value at each nodal point. By this approximation, we can regard the elements of \mathbf{R}^{NP} as the approximate comparison function. Thirdly, calculate the gradient of $J_m(u)$ in \mathbf{R}^{NP} and find a minimum point along the line with the direction $\nabla J_m(u)$. Repeat this step until satisfies the given terminate conditions.

As the usual finite elements method, we calculate the value of integral by summing up the values of each element. For this purpose, we use a volume coordinate to calculate the second term of (1.1) and the first term of (1.2).

6. Numerical examples (Ginzburg-Landau type problem)

We choose $f(u) = \frac{1}{\delta}(|u|^2 - 1)^2$. We treat the case when $n = N = 2$, $\Omega = \mathbf{B}^2$ in (1.2). We are interested in the behavior of zeros and vortices.

Let p_i ($i = 2, 3$), f_z be functions $\mathbf{B}^2 \mapsto \mathbf{R}^2$ such that, for $(x, y) \in \mathbf{B}^2$,

$$p_2(x, y) = \left(\frac{x^2 - y^2}{\sqrt{x^2 + y^2}}, \frac{2xy}{\sqrt{x^2 + y^2}} \right)$$

$$p_3(x, y) = \left(\frac{4x^3 - 3x}{\sqrt{x^2 + y^2}}, \frac{3y - 4y^3}{\sqrt{x^2 + y^2}} \right)$$

and

$$f_z(x, y) = \left((1 - \sqrt{x^2 + y^2})z_1 + x, (1 - \sqrt{x^2 + y^2})z_2 + y \right)$$

for $z = (z_1, z_2) \in \mathbf{B}^2$.

We calculated examples in the following conditions:

	Initial data $u_0(x, y)$	Boundary condition $u_m(x) _{\partial\mathbf{B}^2}$	Parameters
EX.1	$p_2(f_z^{-1}(x, y))$ $z = (-2/5, 0)$	$p_2(x, y) _{\partial\mathbf{B}^2}$	$h = 0.02, \delta = 0.1$
EX.2	$p_3(f_z^{-1}(x, y))$ $z = (-3/7, 0)$	$p_3(f_z^{-1}(x, y))$	The same as EX.1

In Ex 1, we choose zero with degree 2. In this case, a zero with degree 2 splits into two zeros with degree 1. In Ex 2, we choose degree 3 boundary condition and initial data which has a zero with degree 3. In this case, in the final state, a zero splits into three zeros with degree 1.

7. Numerical example (Free boundary problem)

We choose

$$f(u) = \chi_{u>0}^\varepsilon = \begin{cases} 1 & ; \varepsilon < u \\ 0 & ; u \leq 0, \end{cases} \quad (7.1)$$

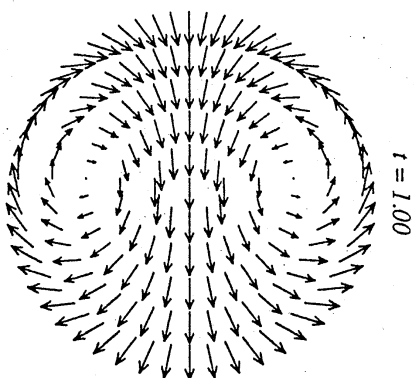
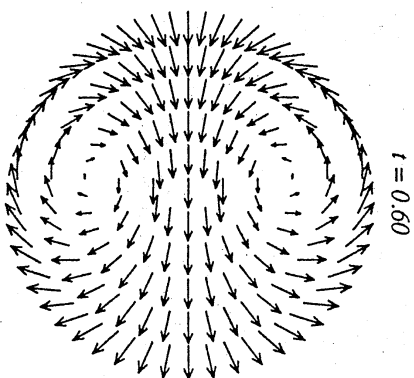
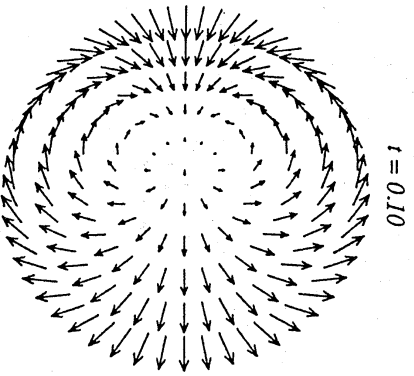
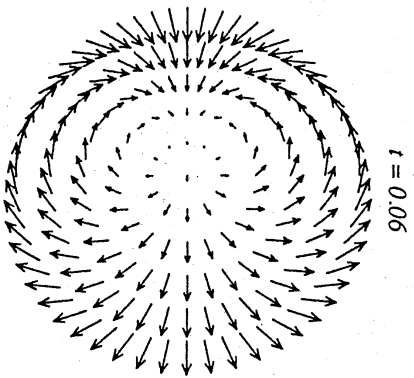
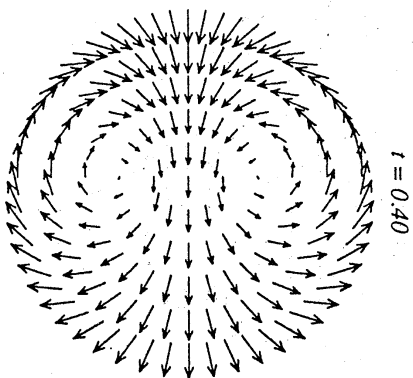
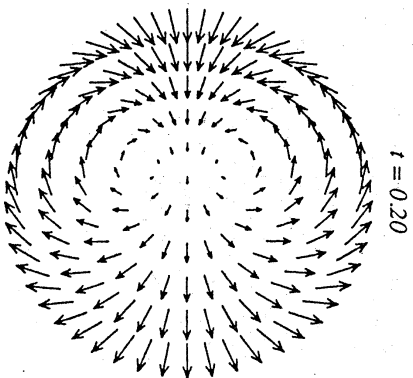
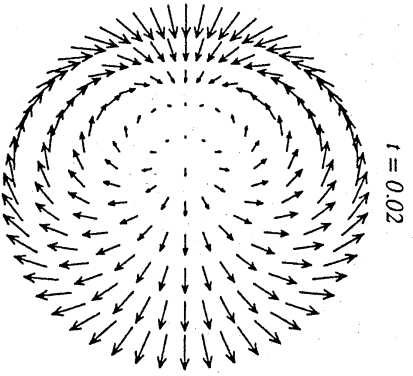
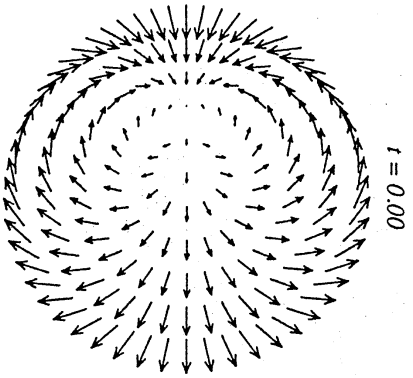
with $\|\nabla \chi_{u>0}^\varepsilon\|_\infty \leq \frac{2}{\varepsilon} \|\nabla u\|_\infty$ and $\chi_{u>0}^\varepsilon \in C^2(\mathbf{R})$. We treat the case $n = 2, N = 1$ and $\Omega = \mathbf{B}^2$.

	Initial data $u_0(x, y)$	Boundary condition $u_m(x) _{\partial\Omega}$	Parameters
Ex.3	$\max(20(\sqrt{x^2 + y^2} - 0.95), 0)$	1.0	$h = 0.005$ $\varepsilon = 0.05$
Ex.4	$\max(7(\sqrt{x^2 + y^2} - 0.95), 0)$	0.35	$h = 0.005$ $\varepsilon = 0.05$

The Ex 3 says that the graph peel off from (x, y) -plane as $t \rightarrow \infty$. On the other hand, in the Ex 4, the graph of u does not completely peeling off from the (x, y) -plane when $t \rightarrow \infty$.

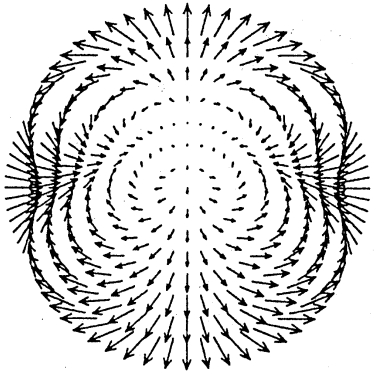
Example 1

$h=0.02, \delta=0.1$

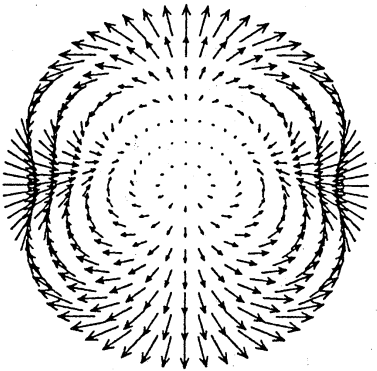


Example 2

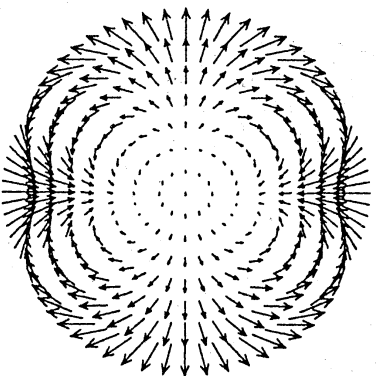
$h=0.02$, $\delta t=0.1$



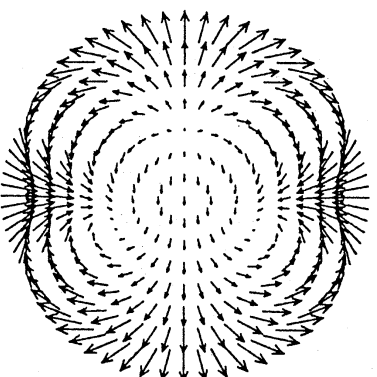
$t = 0.00$



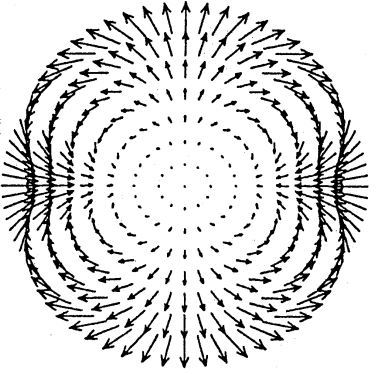
$t = 0.02$



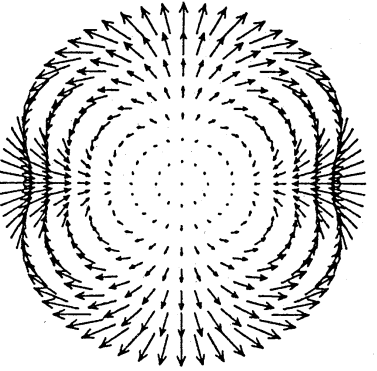
$t = 0.50$



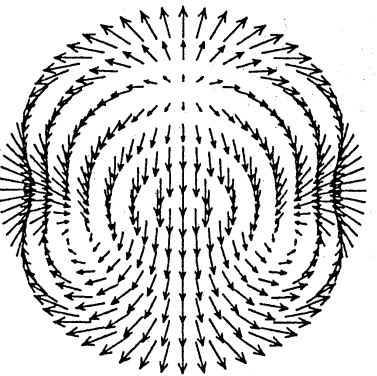
$t = 0.60$



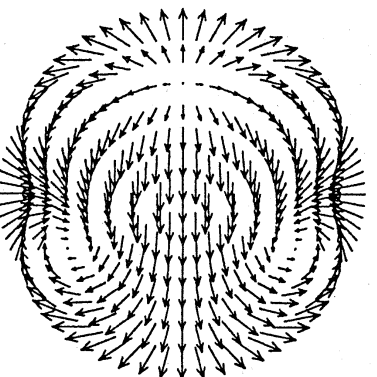
$t = 0.20$



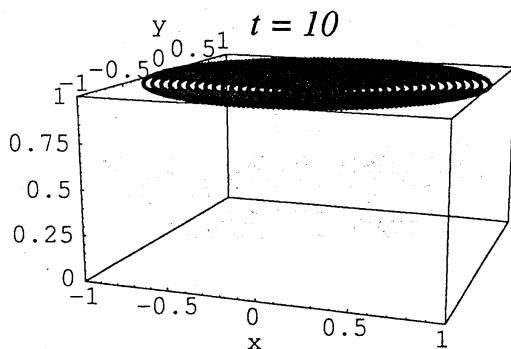
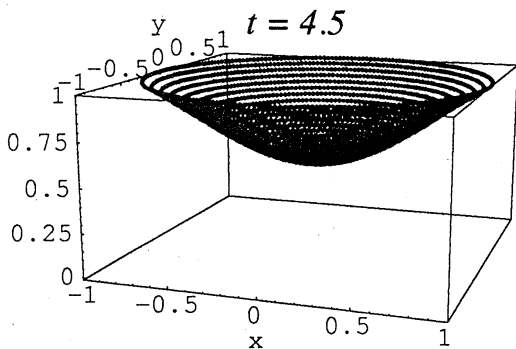
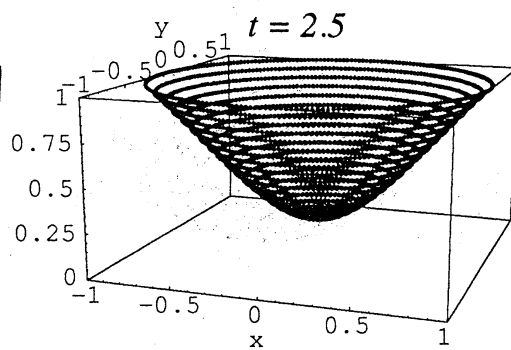
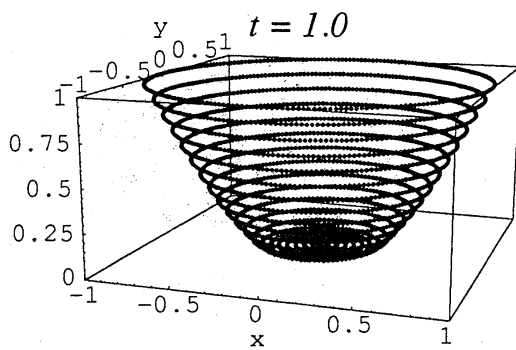
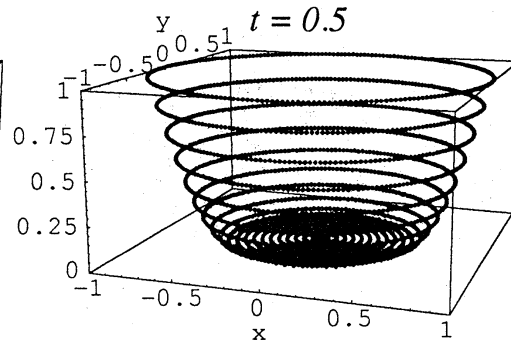
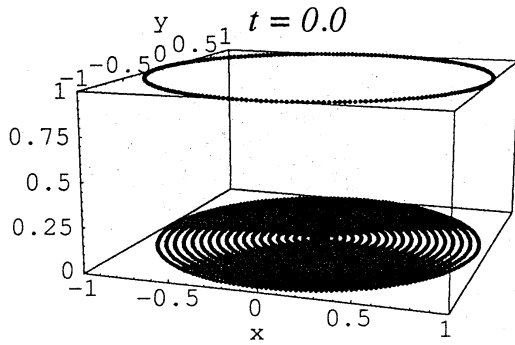
$t = 0.40$



$t = 0.80$

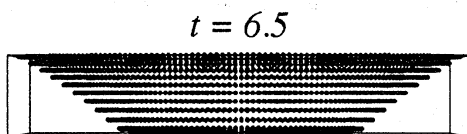
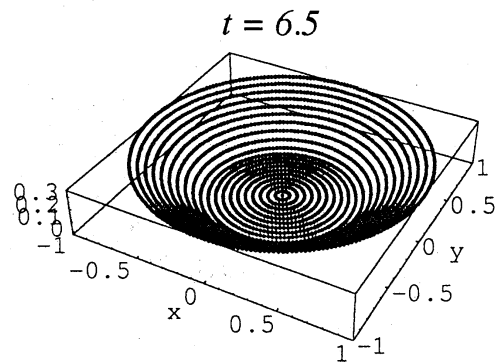
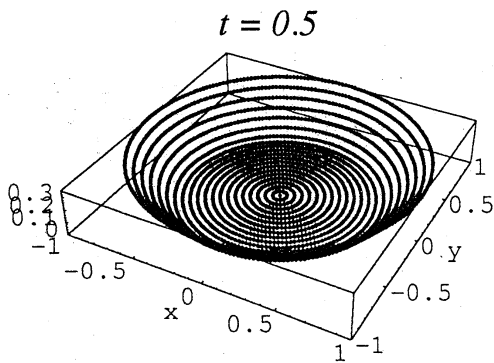
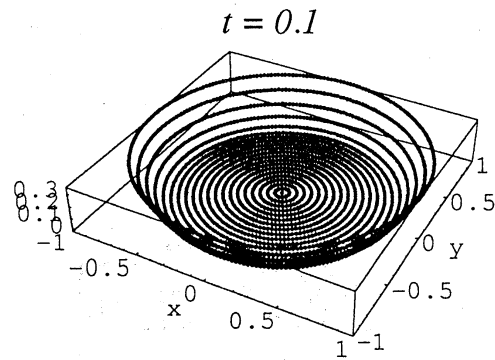
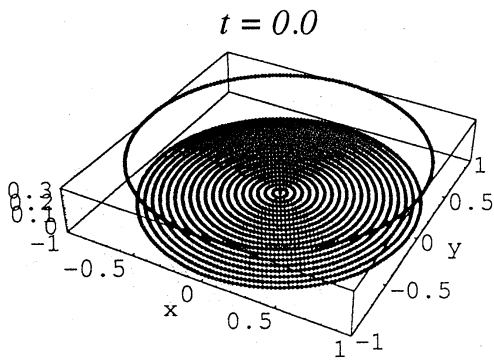


$t = 1.00$

Example 3 **$h=0.005$, $\epsilon=0.05$, $u=1.0$ on the boundary**

Example 4

$h=0.005$, $\epsilon=0.05$, $u=0.35$ on the boundary



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