Estimates and Computations for Melting and Solidification Problems

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Abstract

In this paper we focus on melting and solidification processes described by phase-field models and obtain rigorous estimates for such processes. These estimates are derived in Section 2 and guarantee the convergence of solutions to non-constant equilibrium patterns. The most basic results conclude with the inequality (2.31). The estimates in the remainder of Section 2 illustrate what obtains if the initial data is progressively more regular and may be omitted on first reading. We also present some interesting numerical simulations which demonstrate the equilibrium structures and the approach of the system to non-constant equilibrium patterns. The novel feature of these calculations is the linking of the small parameter in the system, δ, to the grid spacing, thereby producing solutions with approximate sharp interfaces. Similar ideas have been used by Caginalp and Sokolovsky [1]. A movie of these simulations may be found at *http:www.math.cmu.edu/math/people/greenberg.html*.

1 Introduction

In this paper we focus on melting and solidification processes described by phase-field models and obtain rigorous estimates for such processes. These estimates are derived in Section 2 and guarantee the convergence of solutions to non-constant equilibrium patterns. The most basic results conclude with the inequality (2.31). The estimates in the remainder of Section 2 illustrate what obtains if the initial data is progressively more regular and may be omitted on first reading. We also present some interesting numerical simulations which demonstrate the equilibrium structures and the approach of the system to non-constant equilibrium patterns. The novel feature of these calculations is the linking of the small parameter in the system, δ, to the grid spacing, thereby producing solutions with approximate sharp interfaces. Similar ideas have been used by Caginalp and Sokolovsky [1].

For the definiteness we focus on the system

$$T_t + (1-p^2)p_t - a^2\Delta T = 0 \quad , \quad (x,y) \in \Omega \tag{1.1}$$

and

$$\alpha\delta p_t - \lambda^2\delta^2\Delta p = \mu T(1-p^2) + p(1-p^2) \quad , \quad (x,y) \in \Omega. \tag{1.2}$$

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Here Δ is the two-dimensional Laplacian, T is the difference between the absolute temperature θ and the nominal melt temperature of the medium θ_m; i.e. $T = \theta - \theta_m$, and p is a nonconservative order parameter. The parameters α, a, and λ are positive and $O(1)$, $0 < \mu \leq 1$, and $0 < \delta \ll 1$. For definiteness we restrict our attention to the case where Ω is the unit square

$$\Omega = \{(x,y) | -1/2 < x, y < 1/2\}. \tag{1.3}$$

On $\partial\Omega$ we assume that

$$\frac{\partial T}{\partial n} = \frac{\partial p}{\partial n} = 0$$

and at $t = 0$ T and p are prescribed.

The reader should note that (1.1) is the balance of energy

$$e_t + \text{div } q = 0$$

where

$$e = \theta_m + T + p - p^3/3 \quad \text{and} \quad q = -a^2 \nabla T.$$

The reader may be concerned that as defined e is not globally monotone increasing in the order parameter p but this is really not an issue since (i) e is monotone increasing in p on [-1,1] and (ii) if the initial data for p satisfies $-1 \leq p(x,y,0^+) \leq 1$, then the same estimate applies for all future times $t > 0$. This last assertion is a direct consequence of (1.2) and the observation that at a local maximum (minimum) of p that $\Delta p \leq 0 (\Delta p \geq 0)$.

The system (1.1) and (1.2) is close to what Penrose and Fife [2,3] and Sekerka et al [4] call a thermodynamically consistent system. If one lets θ denote the absolute temperature and θ_m denote the nominal melt temperature of the solid, then our internal energy, expressed as a function of θ and p, may be written as

$$e = \theta + p - \frac{p^3}{3}$$

and the Helmholtz free energy, $F(\theta, p)$, satisfies

$$\theta^2 \frac{\partial}{\partial \theta}\left(\frac{F}{\theta}\right) = -e = -\theta - \left(p - \frac{p^3}{3}\right)$$

and

$$F(\theta_m, p) = \frac{(1-p^2)^2}{4}.$$

These latter two conditions imply that

$$F(\theta, p) = \frac{\theta}{4\theta_m}(1-p^2)^2 + \frac{1}{\theta_m} ln\left(\frac{\theta_m}{\theta}\right) - \frac{(\theta - \theta_m)}{\theta_m}\left(p - p^3/3\right)$$

and the thermodynamically consistent phase-field equation for p associated with F is

$$\tilde{\alpha}\delta p_t - \tilde{\lambda}^2\delta^2\Delta p = -\frac{1}{\theta}\frac{\partial F}{\partial p} = \left(\frac{\theta-\theta_m}{\theta\theta_m} + \frac{p}{\theta_m}\right)\left(1-p^2\right).$$

where $\tilde{\alpha} = \dfrac{\alpha}{\theta_m}$ and $\tilde{\lambda} = \dfrac{\lambda}{(\theta_m)^{1/2}}$. This latter equation, together with $\theta = \theta_m + T$, implies that the above consistent phase-field equation reduces to (1.2) with $\mu = \dfrac{1}{\theta_m}$ in the limit where $T \to 0$.

There are a variety of similar phase-field models which have been studied. Many of these may be written succinctly as

$$T_t + \left(1-p^2\right)^n p_t = a^2\Delta T = 0 \tag{1.4}$$

and

$$\alpha\delta p_t - \lambda^2\delta^2\Delta p = \mu T\left(1-p^2\right)^m + p\left(1-p^2\right) \tag{1.5}$$

where n and m are non-negative integers.

In [5-7] Caginalp focused primarily on the case where $n = m = 0$. In [8] Caginalp and Chen considered (1.4) and (1.5) when $n = 0$ and $m = 2$. The case where $n = m = 2$ has been studied by Sekerka and collaborators in [9,10]. The situation where $n = m = 0$ is slightly different than when n and m are both ≥ 1 because the latter situation loses the pointwise estimates $-1 \leq p(x,y,t) \leq 1$. Fabbri and Vollmer [11] have also noted this difference.

All of these models yield a diffuse interface description of melting and solidification. Corresponding to each particular model there is a corresponding sharp-interface description which is obtained by letting δ tend to 0^+. For the system (1.1) and (1.2) the sharp-interface description takes the following simple form. p takes on only the values -1 and +1. Solid regions are those where $p = -1$ and liquid regions those where $p = +1$. In what follows

$$\Gamma(t) = \{(x,y) \mid x = \hat{x}(s,t),\ y = \hat{y}(s,t),\ 0 \leq s \leq L\} \tag{1.6}$$

will be a curve separating liquid and solid regions and $\boldsymbol{n}(s,t)$ will be the unit normal to Γ which points into the liquid region. The unit tangent, $\boldsymbol{t}$, to Γ is chosen so that $\boldsymbol{n}(s,t) \times \boldsymbol{t}(s,t) = \boldsymbol{e}_3$. K is the curvature of Γ at $(\hat{x},\hat{y})(s,t)$, and

$$c(s,t) \stackrel{def}{=} (\hat{x}_t,\ \hat{y}_t)\cdot\boldsymbol{n}(s,t) \tag{1.7}$$

is the speed at which Γ moves in the direction $\boldsymbol{n}$. A singular perturbation analysis of (1.1) and (1.2) yields the following results:

1. T is continuous across Γ;

2. On Γ the Gibbs-Thomson relation

$$\alpha c + \lambda^2 \delta K = -2^{1/2} \lambda \mu T_M \tag{1.8}$$

holds; and finally across Γ (1.1) implies that

$$\frac{4}{3} c = a^2 \left(\frac{\partial T^-}{\partial n} - \frac{\partial T^+}{\partial n} \right). \tag{1.9}$$

In (1.8), $T_M(s) = T\left(\hat{x}(s,t),\ \hat{y}(s,t)\right)$, is the local melt temperature while in (1.9) $\dfrac{\partial T^+}{\partial n}$ is the normal derivative of T in the liquid region and $\dfrac{\partial T^-}{\partial n}$ is the normal derivative of T in the solid region. In the sharp-interface description one solves the heat equation

$$T_t - a^2 \Delta T = 0$$

in the portion of Ω away from interfaces. At equilibrium, $c = 0$ and (1.8) implies that $T_M = O(\delta)$. In what follows, we shall restrict our attention to initial data $T(x, y, 0^+)$ that is at worst $O(\delta^{\frac{1}{2}})$.

The sharp-interface description becomes unduly complicated in the presence of multiple interfaces since all must be tracked. Difficulties also arise when interfaces merge. For these, and a plethora of other reasons, we focus on (1.1) and (1.2). Our principal results consist of a sequence of a-priori inequalities satisfied by solutions of the system (1.1) and (1.2). These estimates guarantee regularity of the solutions and that the solutions converge to non-constant equilibria as t tends to infinity.

One point worthy of note is that it is possible to obtain solutions of (1.1) and (1.2) which approximate those generated by the sharp interface descriptions. These are produced by solving (1.1) and (1.2) with initial data $p^\delta(x, y, 0^+)$ which approximate the jump discontinuous data of the sharp interface theory but transition smoothly from -1 to $+1$ over an interval of width of $O(\delta)$ in the direction $\boldsymbol{n}$. For such initial p's (and initial temperature fields satisfying $T(x, y, 0^+) = O(\delta^{\frac{1}{2}})$) we are guaranteed that terms like $\delta \int\int_\Omega | \bigtriangledown p^\delta|^2 dxdy$ and $\frac{1}{\delta} \int\int_\Omega (1 - p^2)^2\, dxdy$ are bounded independently of δ and t. These are the estimates which link the solutions of the two theories.

We note there is an "intermediate" model with the same equilibrium as the full system (1.1) and (1.2). In the "intermediate" model one replaces the local energy equation with the following identity for the average temperature:

$$T_0(t) = h_0 - \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(p - p^3/3\right)(x, y, t)dxdy \tag{1.10}$$

and solves

$$\alpha \delta p_t - \lambda^2 \delta^2 \Delta p = (\mu T_0 + p)\left(1 - p^2\right),\ (x, y) \in \Omega \tag{1.11}$$

and

$$\frac{\partial p}{\partial n}=0 \quad , \quad (x,y)\in\partial\Omega. \tag{1.12}$$

The constant h_0 in (1.10) is calculated from the initial data for the full system by

$$h_0=\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(T+p-p^3/3\right)(x,y,0^+)dxdy. \tag{1.13}$$

This "intermediate" model is justified by two facts. The first is that solutions of (1.1) and (1.2) satisfying the boundary conditions $\frac{\partial T}{\partial n}=\frac{\partial p}{\partial n}=0,\ (x,y)\in\partial\Omega$ satisfy the overall balance equation

$$h_0\equiv\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(T+p-p^3/3\right)(x,y,t)dxdy \tag{1.14}$$

for all $t\geq 0$ and the second is that the spatially varying portion of T decays to zero as t tends to infinity (for details see the comments following (2.17)). The second observation allows us to replace the local temperature in (1.2) by the spatial average defined in (1.10).

2 Entropies and A-Priori Estimates

Our goal in this section is a set of inequalities of the form

$$\frac{\partial\eta}{\partial t}-\text{div }\boldsymbol{q}\leq G \tag{2.1}$$

satisfied by solutions of

$$T_t+\left(1-p^2\right)p_t-a^2\Delta T=0 \quad , \quad (x,y)\in\Omega, \tag{2.2}$$

$$\alpha\delta p_t-\lambda^2\delta^2\Delta p=(\mu T+p)\left(1-p^2\right),\ (x,y)\in\Omega, \tag{2.3}$$

and

$$\frac{\partial T}{\partial n}=\frac{\partial p}{\partial n}=0\ ,\ (x,y)\in\partial\Omega. \tag{2.4}$$

Once again

$$\Omega=\{(x,y)\mid -1/2<x<1/2 \text{ and } -1/2<y<1/2)\}. \tag{2.5}$$

For (2.1) to be of value we require

$$0 \leq \eta,\ (x,y) \in \Omega \text{ and } \boldsymbol{q} \cdot \boldsymbol{n} = 0,\ (x,y) \in \partial\Omega \tag{2.6}$$

and that either $G \leq 0$ in Ω or G is a-priori bounded in $L_1(\Omega \times (0,\infty))$. Throughout we exploit the pointwise estimates

$$-1 \leq p(x,y,t) \leq 1\ ,\ (x,y) \in \Omega \text{ and } t \geq 0 \tag{2.7}$$

satisfied by solutions of (2.3).

Once again we record the overall energy balance satisfied by solutions of (2.2) – (2.4), namely the identity:

$$\int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(T + p - p^3/3\right)(x,y,t)dxdy \equiv h_0. \tag{1.13}$$

This is obtained by integrating (2.2) over Ω and exploiting $(2.4)_1$.

Our first inequality is obtained by multiplying (2.2) by $\left(\frac{\mu T}{\delta}\right)$ and (2.3) by $\frac{p_t}{\delta}$ and adding the resulting identities. This yields (2.1) with

$$\eta_1 = \frac{\mu T^2}{2\delta} + \frac{\lambda^2\delta}{2}| \bigtriangledown p|^2 + \frac{\left(1-p^2\right)^2}{4\delta}, \tag{2.8}$$

$$\boldsymbol{q}_1 = \frac{\mu a^2}{\delta} T \bigtriangledown T + \lambda^2 \delta p_t \bigtriangledown p, \tag{2.9}$$

and

$$G_1 = -\alpha p_t^2 - \frac{\mu a^2 | \bigtriangledown T|^2}{\delta} \tag{2.10}$$

and (2.8)-(2.10) yield

$$\begin{aligned} &\frac{d}{dt}\int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(\frac{\mu T^2}{2\delta} + \frac{\lambda^2\delta}{2}| \bigtriangledown p|^2 + \frac{\left(1-p^2\right)^2}{4\delta}\right)(x,y,t)dxdy \\ &\leq -\int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(\alpha p_t^2 + \frac{\mu a^2}{\delta}| \bigtriangledown T|^2\right)(x,y,t)dxdy. \end{aligned} \tag{2.11}$$

Once again we restrict our attention to initial data satisfying

$$\int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(\frac{T^2}{2\delta} + \frac{\lambda^2\delta}{2}| \bigtriangledown p|^2 + \frac{\left(1-p^2\right)^2}{4\delta}\right)(x,y,0^+)dxdy = 0(1)$$

independent of δ.

If we next multiply (2.2) by αT_t we obtain

$$\frac{\alpha a^2}{2}\frac{\partial}{\partial t}|\bigtriangledown T|^2 - \alpha a^2 \text{ div } (T_t \bigtriangledown T) = -\alpha\left(T_t^2 + \left(1-p^2\right) p_t T_t\right)$$

and if we add this result to (2.1) with $\eta_1,\ \boldsymbol{q}_1,\ G_1$ we obtain

$$\frac{\partial \eta_2}{\partial t} - \text{div } \boldsymbol{q}_2 \le G_2$$

where

$$\eta_2 = \frac{\mu T^2}{2\delta} + \frac{\lambda^2\delta}{2}|\bigtriangledown p|^2 + \frac{\left(1-p^2\right)^2}{4\delta} + \frac{\alpha a^2}{2}|\bigtriangledown T|^2 \tag{2.12}$$

$$\boldsymbol{q}_2 = \frac{\mu a^2}{\delta} T \bigtriangledown T + \lambda^2 \delta p_t \bigtriangledown p + \alpha a^2 T_t \bigtriangledown T \tag{2.13}$$

and

$$G_2 = -\alpha\left(p_t^2 + T_t^2 + \left(1-p^2\right) T_t p_t\right) - \frac{\mu a^2}{\delta}|\bigtriangledown T|^2 \le \frac{-\alpha}{2}\left(p_t^2 + T_t^2\right) - \frac{\mu a^2}{\delta}|\bigtriangledown T|^2 \tag{2.14}$$

and (2.12)-(2.14) imply that

$$\begin{aligned}&\frac{d}{dt}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(\frac{\mu T^2}{2\delta} + \frac{\lambda^2\delta}{2}|\bigtriangledown p|^2 + \frac{\left(1-p^2\right)^2}{4\delta} + \frac{\alpha a^2}{2}|\bigtriangledown T|^2\right)(x,y,t)dxdy \\ &\le -\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(\frac{\alpha}{2}\left(p_t^2 + T_t^2\right) + \frac{\mu a^2}{\delta}|\bigtriangledown T|^2\right)(x,y,t)dxdy.\end{aligned} \tag{2.15}$$

If we now write

$$T(x,y,t) = T_0(t) + T_1(x,y,t) \quad , \quad (x,y) \in \Omega \tag{2.16}$$

where

$$T_0(t) \equiv \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} T(x,y,t)dxdy \text{ and } \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} T_1(x,y,t)dxdy \equiv 0, \tag{2.17}$$

then (2.15) implies that if T and p are in $H^1(\Omega)$ at $t=0$, then they are in $H^1(\Omega)$ for all $t>0$ and that T satisfies $\lim\limits_{t\to\infty}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} T_1^2(x,y,t)dxdy = 0$.

If we make a similar decomposition of p, that is write

$$p(x,y,t) = p_0(t) + p_1(x,y,t) \tag{2.18}$$

where

$$p_0(t) \equiv \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} p(x,y,t)dxdy \text{ and } \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} p_1(x,y,t)dxdy \equiv 0, \tag{2.19}$$

then (2.3) implies that

$$\alpha\delta\frac{dp_0}{dt} = \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} (\mu T + p)(1-p^2)(x,y,t)dxdy \tag{2.20}$$

and

$$\alpha\delta\frac{d^2p_0}{dt^2} = \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} \left(\mu\left(T_t\left(1-p^2\right) - 2pTp_t\right) + \left(1-3p^2\right)p_t\right)(x,y,t)dxdy \tag{2.21}$$

and (2.20) and (2.21) along with the fact that (2.15) implies that p_t and T_t are $L_2(\Omega\times(0,\infty))$ combine to yield the result that $\frac{dp_0}{dt}$ and $\frac{d^2p_0}{dt^2}$ are in $L_2(0,\infty)$ and that

$$\lim_{t\to\infty}\alpha\delta\frac{dp_0}{dt} = \lim_{t\to\infty}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} (\mu T + p)(1-p^2)(x,y,t)dxdy = 0. \tag{2.22}$$

With the estimate (2.15) we can derive weak information about the long-term behavior of solutions of (2.2)-(2.4). In what follows we let

$$(T^t, p^t)(x,y,s) = (T,p)(x,y,t+s),\ \ (x,y)\in\Omega \text{ and } 0\le s\le s_*. \tag{2.23}$$

The inequality (2.15), together with (2.7), implies that for any s_* the functions T^t and p^t are in $H^1(\Omega\times(0,s_*))$ with bounds which depend only on the $H^1(\Omega)$ norms of $T(x,y,0^+)$ and $p(x,y,0^+)$ and s_* and that

$$\lim_{t\to\infty}\int_0^{s_*}\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(\frac{\alpha}{2}\left(\left(T_s^t\right)^2 + \left(p_s^t\right)^2\right) + \frac{\mu a^2}{\delta}|\bigtriangledown T^t|^2\right)(x,y,s)dxdy\right)ds = 0. \tag{2.24}$$

Moreover, (2.3) implies that $\lambda^2\delta^2\Delta p^t \in L_2(\Omega\times(0,s_*))$ with bounds which are independent of t. The boundedness of T^t and p^t in $H^1(\Omega\times(0,s_*))$ implies we can find an increasing sequence $\{t_i\}_{i=1}^\infty$ with $\lim_{i\to\infty} t_i = \infty$ and functions T^∞ and p^∞ in $H^1(\Omega\times(0,s_*))$ with Δp^∞ in $L_2(\Omega\times(0,s_*))$ with the following properties:

(T^∞, p^∞) is the strong $L_2(\Omega \times (0, s_*))$ limit of (T^{t_i}, p^{t_i}) while T_s^∞, $p_s^\infty, \bigtriangledown T^\infty, \bigtriangledown p^\infty$, and Δp^∞ are the weak $L_2(\Omega \times (0, s_*))$ limits of the appropriate derivatives of T^{t_i} and p^{t_i}. Additionally, (2.24) implies

$$T_s^\infty = p_s^\infty = 0 \text{ and } \bigtriangledown T^\infty = 0 \text{ in } \Omega \times (0, s_*) \tag{2.25}$$

and thus that T^∞ is a constant and p^∞ is independent of s. The energy balance (1.13) yields

$$T^\infty = h_0 - \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(p^\infty - (p^\infty)^3/3\right)(x, y) dx dy \tag{2.26}$$

while (2.7) implies that $-1 \le p^\infty \le 1$. (2.3) and (2.24) also imply that p^∞ satisfies the equilibrium equation

$$\lambda^2 \delta^2 \Delta p^\infty + (\mu T^\infty + p^\infty)\left(1 - (p^\infty)^2\right) = 0, \ (x, y) \in \Omega \tag{2.27}$$

and

$$\frac{\partial p^\infty}{\partial n} = 0, \ (x, y) \in \partial\Omega \tag{2.28}$$

where T^∞ is given by (2.26). Moreover, (2.27) and (2.28) imply that p^∞ is a critical point of the functional

$$N(p^\infty) \stackrel{def}{=} \frac{\mu (T^\infty)^2}{2\delta} + \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(\frac{\lambda^2 \delta}{2} | \bigtriangledown p^\infty|^2 + \frac{\left(1 - (p^\infty)^2\right)^2}{4\delta} \right)(x, y) dx dy \tag{2.29}$$

and that

$$\eta(t, s_*) \stackrel{def}{=} \frac{1}{s_*} \int_0^{s_*} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(\frac{\mu (T^t)^2}{2\delta} + \frac{\lambda^2 \delta}{2} | \bigtriangledown p^t|^2 + \frac{\left(1 - (p^t)^2\right)^2}{4\delta} + \frac{\alpha a^2}{2} | \bigtriangledown T^t|^2 \right)(x, y, s) dx dy ds \tag{2.30}$$

is decreasing in t and has a limit η_∞ satisfying

$$N(p^\infty) \le \eta_\infty \le \eta(0^+) = O(1). \tag{2.31}$$

The last inequality guarantees that if the constant h_0 defined in (1.13) is small enough then p^∞ is not identically constant. For simplicity we demonstrate this when $h_0 = 0$ and when the initial data for T is the constant

$$T(x,y,0^+) = \iint_\Omega (p - p^3/3)(x,y,0^+)dx\,dy.$$

We also assume that $p(\cdot,\cdot,0^+)$ is such that $T(\cdot,\cdot,0^+) = O(\delta^{1/2})$ and that $\iint_\Omega \eta_2(x,y,0^+)dx\,dy = O(1)$ (see (2.12)). These constraints on the data guarantee that the limit $\eta + \infty$ in (2.30) is $O(1)$.

If we now suppose that p^∞ is constant on Ω, then $N(p^\infty)$ reduces to

$$F(p^\infty) = \frac{\mu}{2\delta}\left(p^\infty - (p^\infty)^3/3\right) + \frac{(1-(p^\infty)^2)}{4\delta}$$

and p^∞ is a critical point of F; i.e., satisfies

$$(1-p^2)\left((\mu-1)p - \frac{p^3}{3}\right) = 0$$

But, the assumption $0 < \mu \leq 1$ guarantees the critical points are $(-1,0,1)$ and the associated critical values are $\left(\frac{2\mu}{9\delta}, \frac{1}{4\delta}, \frac{2\mu}{9\delta}\right)$. For $0 < \delta \ll 1$, all of these critical values are greater than η_∞ and this, along with (2.31), confirms that the limits we obtain are non-constant equilibria.

To obtain stronger information we examine the time differentiated versions of (2.2)-(2.4), namely the equations:

$$T_{tt} + (1-p^2)p_{tt} - 2pp_t^2 - a^2\Delta T_t - 0,\ (x,y) \in \Omega, \tag{2.32}$$

$$\alpha\delta p_{tt} - \lambda^2\delta^2\Delta p_t = (\mu T_t + p_t)(1-p^2) - 2p(\mu T + p)p_t,\ (x,y) \in \Omega, \tag{2.33}$$

$$\frac{\partial T_t}{\partial n} = \frac{\partial p_t}{\partial n} = 0 \quad , \quad (x,y) \in \partial\Omega. \tag{2.34}$$

We shall also exploit

Lemma 1. Suppose $f \in H^1(\Omega)$. Then, for every $\epsilon > 0$

$$\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} f^4(x,y)dxdy \leq 4\left[\frac{(1+\epsilon)}{\epsilon}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} f^2(x,y)dxdy + \epsilon\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} |\bigtriangledown f|^2(x,y)dxdy\right]^2.$$

We multiply (2.33) by p_t and make use of (2.7) to obtain

$$\frac{\alpha\delta}{2}\frac{\partial}{\partial t}p_t^2 - \lambda^2\delta^2 \operatorname{div}\,(p_t \bigtriangledown p_t) \leq -\lambda^2\delta^2|\bigtriangledown p_t|^2 + \left(\frac{\mu T_t^2}{2} + \left(1 + \frac{\mu}{2}\right)p_t^2\right) + 2\mu|T|p_t^2. \tag{2.35}$$

We note that (2.15) implies the term $\dfrac{\mu {T_t}^2}{2} + \left(1+\dfrac{\mu}{2}\right)p_t^2$ is in $L_1(\Omega \times (0,\infty))$ and thus we confine our attention to $2\mu|T|p_t^2$. Schwarz's inequality and Lemma 1 imply

$$2\mu\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(|T|p_t^2\right)(x,y,t)dxdy \leq 2\mu\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}T^2(x,y,t)dxdy\right)^{1/2}\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^4(x,y,t)dxdy\right)^{1/2}$$

$$\leq 2\mu\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}T^2(x,y,t)dxdy\right)^{1/2}\left(\left(\frac{1+\epsilon}{\epsilon}\right)\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2(x,y,t)dxdy+\epsilon\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p_t|^2(x,y,t)dxdy\right).$$

Moreover, (2.11) guarantees that

$$\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}T^2(x,y,t)dxdy\right)^{1/2} \leq \left(\frac{2\delta}{\mu}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\eta_1(x,y,0^+)dxdy\right)^{1/2} \qquad (2.36)\ (2.37)$$

and this guarantees that we may choose ϵ so that

$$2\mu\epsilon\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}T^2(x,y,t)dxdy\right)^{1/2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p_t|^2(x,y,t) \leq \frac{\lambda^2\delta^2}{2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p_t|^2(x,y,t)dxdy. \tag{2.38}$$

With ϵ so chosen, (2.35) implies that

$$\frac{\alpha\delta}{2}\frac{d}{dt}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2(x,y,t) \leq \frac{-\lambda^2\delta^2}{2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p_t|^2(x,y,t)dxdy + \frac{\mu}{2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}T_t^2(x,y,t)dxdy$$
$$+\left(1+\frac{\mu}{2}+2^{3/2}\left(\mu\delta\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\eta_1(x,y,0^+)dxdy\right)^{1/2}\left(1+\frac{1}{\epsilon}\right)\right)\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2(x,y,t)dxdy \tag{2.39}$$

and (2.39) then implies that if

$$p_t(x,y,0^+) = \frac{1}{\alpha\delta}\left(\lambda^2\delta^2\Delta p + (\mu T + p)(1-p^2)\right)(x,y,0^+)$$

is in $L_2(\Omega)$, then p_t and thus Δp are in $L_2(\Omega)$ independently of t and $\bigtriangledown p_t \in L_2(\Omega \times (0,\infty))$.

The preceding estimate points up the advantage of the "intermediate" model discussed briefly in (1.9)-(1.12) over the full system. For the intermediate model the cantankerous term $2\mu|T|p_t^2$ in (2.35) would have been replaced by $2\mu|T_0|p_t^2$ and this latter term is easily controlled since we know by our previous estimates that

$$|T_0| \leq \left(\frac{2\delta}{\mu}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\eta_1(x,y,0^+)dxdy\right)^{1/2}$$

and thus we would not have to invoke Lemma 1 and choose $\epsilon = 0\left(\delta^{3/2}\right)$. This latter choice of ϵ pumped up the coefficient of $\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} p_t^2(x,y,t)dxdy$ in (2.39) to be $O\left(1/\delta^{3/2}\right)$ which is far from optimal. If we chose to add some multiple of (2.39) to (2.15) and wanted the right hand side of the resulting inequality to be negative definite our multiplier would have to be $O(\delta^{3/2})$, an unacceptably small number. For the "intermediate" model we could use an $O(1)$ multiplier (for details see (2.61)-(2.63)).

On the other hand, if we multiply (2.32) by $(T_t + (1-p^2)p_t)/a^2$ we find that

$$\begin{aligned} &\frac{1}{2a^2}\frac{\partial}{\partial t}\left(T_t + (1-p^2)p_t\right)^2 = \frac{a^2}{2}\frac{\partial}{\partial t}(\Delta T)^2 \\ &= \text{div}\ \left((T_t + (1-p^2)p_t) \bigtriangledown T_t\right) - |\bigtriangledown T_t|^2 - (1-p^2)\bigtriangledown T_t \cdot \bigtriangledown p_t + 2pp_t \bigtriangledown T_t \cdot \bigtriangledown p \end{aligned} \tag{2.40}$$

and (2.40) implies that

$$\begin{aligned} &\frac{a^2}{2}\frac{d}{dt}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}(\Delta T)^2(x,y,t)dxdy \leq \\ &-\frac{1}{2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown T_t|^2(x,y,t)dxdy + \int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p_t|^2(x,y,t)dxdy \\ &+4\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2|\bigtriangledown p|^2(x,y,t)dxdy. \end{aligned} \tag{2.41}$$

The first term on the right hand side of (2.41) is in controllable by virtue of the minus sign and the second term is $L_1(0,\infty)$ by virtue of (2.39). Thus we can confine our attention to the third term. To show this term is $L_1(0,\infty)$ we note that

$$\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2|\bigtriangledown p|^2(x,y,t)dxdy \leq \left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^4(x,y,t)dxdy\right)^{1/2}\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p|^4(x,y,t)dxdy\right)^{1/2}. \tag{2.42}$$

Lemma 1 then guarantees that

$$\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^4(x,y,t)dxdy\right)^{1/2} \leq (1+\sqrt{5})\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(p_t^2 + |\bigtriangledown p_t|^2\right)(x,y,t)dxdy\right) \tag{2.43}$$

and that

$$
\begin{aligned}
&\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} |\bigtriangledown p|^4(x,y,t)dxdy\right)^{1/2} \\
\leq\ & 2^{1/2}\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} p_x^4(x,y,t)dxdy\right)^{1/2} + 2^{1/2}\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} p_y^4(x,y,t)dxdy\right)^{1/2} \\
\leq\ & 2^{1/2}\left(1+\sqrt{5}\right)\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(p_x^2+p_y^2+p_{xx}^2+p_{yy}^2+2p_{xy}^2\right)(x,y,t)dxdy \\
\leq\ & 2^{1/2}\left(1+\sqrt{5}\right)\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(p_x^2+p_y^2+(\Delta p)^2\right)(x,y,t)dxdy
\end{aligned}
\tag{2.44}
$$

and (2.43) and (2.44) together with (2.41) guarantee that if $T(x,y,0^+)$ and $p(x,y,0^+)$ are in $H^2(\Omega)$ then $T(x,y,t)$ is in $H^2(\Omega)$ for all future times and additionally that $\bigtriangledown T_t \in L_2(\Omega \times (0,\infty))$.

The estimates (2.39) and (2.44) also guarantee that if $T(x,y,0^+)$ and $p(x,y,0^+)$ are in $H^2(\Omega)$, then the resulting orbit is compact in $H^1(\Omega)$ and that the w-limit set is nonempty in $H^1(\Omega)$. The fact that $\bigtriangledown T_t \in L_2(\Omega\times(0,\infty))$ further guarantees that the function T_1 defined in (2.16) and (2.17) converges to zero strongly in $H^1(\Omega)$.

Our final estimates pertain to solutions generated by initial data $T(x,y,0^+)\in H^2(\Omega)$ and $p(x,y,0^+)\in H^3(\Omega)$. These are obtained by multiplying (2.33) by p_{tt}. The resulting inequality is

$$
\begin{aligned}
&\frac{\lambda^2\delta^2}{2}\frac{\partial}{\partial t}|\bigtriangledown p_t|^2 + \alpha\delta p_{tt}^2 - \lambda^2\delta^2 \text{ div } \left(p_{tt}\bigtriangledown p_t\right) = \\
&\mu\left(T_t(1-p^2)-2pTp_t\right)p_{tt} + (1-3p^2)p_tp_{tt} \\
&\leq \frac{\alpha\delta}{2}p_{tt}^2 + \frac{2\mu^2}{\alpha\delta}\left(T_t^2+4T^2p_t^2\right) + \frac{8}{\alpha\delta}p_t^2.
\end{aligned}
\tag{2.45}
$$

Our preceding calculations imply that if $T(x,y,0^+)\in H^2(\Omega)$ and $p(x,y,0^+)\in H^3(\Omega)$, then

$$
\frac{2\mu^2}{\alpha\delta}\left(T_t^2+4T^2p_t^2\right)+\frac{8}{\alpha\delta}p_t^2
$$

is in $L_1(\Omega\times(0,\infty))$ and thus (2.45) implies that $\bigtriangledown p_t \in L_2(\Omega)$ independently of t and that $p_{tt}\in L_2(\Omega\times(0,\infty))$. The former conclusion, together with (2.3), implies that $p\in H^3(\Omega)$ with bounds which are independent of t while the latter conclusion implies that

$$
\lim_{t\to\infty}\alpha\delta p_t = \lim_{t\to\infty}\left(\lambda^2\delta^2\Delta p + (\mu T + p)(1-p^2)\right) = 0
$$

and that this limit is obtained strongly in $L_2(\Omega)$.

We conclude this section with some observations about the "intermediate" model introduced in (1.9)-(1.12). Once again in that model one replaces (2.3) with

$$\alpha\delta p_t - \lambda^2\delta^2\Delta p = (\mu T_0 + p)(1-p^2), (x,y) \in \Omega \tag{2.46}$$

and

$$\frac{\partial p}{\partial n} = 0 \quad , \quad (x,y) \in \partial\Omega \tag{2.47}$$

where

$$T_0(t) = h_0 - \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} \left(p - p^3/3\right)(x,y,t)dxdy \text{ and } h_0 = \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} \left(T + p - p^3/3\right)(x,y,0^+)dxdy. \tag{2.48}$$

Solutions of this latter system also satisfy the pointwise estimates $-1 \leq p(x,y,t) \leq 1$ and a set of "entropy" inequalities similar to those satisfied by solutions of the full system. The most basic of these is

$$\frac{\partial \tilde{\eta}_1}{\partial t} - \text{div } \tilde{\boldsymbol{q}}_1 = \tilde{G}_1 \tag{2.49}$$

where

$$\tilde{\eta}_1 = \frac{\mu T_0^2}{2\delta} + \frac{\lambda^2\delta}{2}| \bigtriangledown p|^2 + \frac{(1-p^2)^2}{4\delta} \tag{2.50}$$

$$\tilde{\boldsymbol{q}}_1 = \lambda^2\delta p_t \bigtriangledown p \tag{2.51}$$

and

$$\tilde{G}_1 = -\alpha p_t^2. \tag{2.52}$$

Moreover, (2.49) - (2.52) imply that

$$\begin{aligned}&\frac{d}{dt}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(\frac{\mu T_0^2}{2\delta} + \frac{\lambda^2\delta}{2}| \bigtriangledown p|^2 + \frac{(1-p^2)^2}{4\delta}\right)(x,y,t)dxdy \\ &\leq -\alpha\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} p_t^2(x,y,t)dxdy.\end{aligned} \tag{2.53}$$

The time differentiated identities

$$\alpha\delta p_{tt} - \lambda^2\delta^2\Delta p_t = \mu\left(\dot{T}_0(1-p^2) - 2pT_0p_t\right) + (1-3p^2)p_t, \tag{2.54}$$

$$\dot{T}_0 = -\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}(1-p^2)p_t(x,y,t)dxdy, \tag{2.55}$$

and

$$\frac{\partial p_t}{\partial n} = 0 \quad , \quad (x,y) \in \partial\Omega. \tag{2.56}$$

also yields:

$$\begin{aligned}
&\frac{\alpha\delta}{2}\frac{\partial p_t^2}{\partial t} - \lambda^2\delta^2 \text{ div } (p_t \bigtriangledown p_t) = \\
&-\lambda^2\delta^2|\bigtriangledown p_t|^2 + \mu\left(\dot{T}_0(1-p^2) - 2pT_0p_t\right)p_t + (1-3p^2)p_t^2 \\
&\leq -\lambda^2\delta^2|\bigtriangledown p_t|^2 + \frac{\mu}{2}\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2(x,y,t)dxdy\right) \\
&+2^{3/2}\mu^{1/2}\delta^{1/2}\left(\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\tilde{\eta}_1(x,y,0^+)dxdy\right)^{1/2}p_t^2 + (1+\frac{\mu}{2})p_t^2
\end{aligned} \tag{2.57}$$

and

$$\begin{aligned}
&\frac{\lambda^2\delta^2}{2}\frac{\partial|\bigtriangledown p_t|^2}{\partial t} - \lambda^2\delta^2 \text{ div } (p_{tt} \bigtriangledown p_t) = \\
&-\alpha\delta p_{tt}^2 + \mu\left(\dot{T}_0(1-p^2) - 2pT_0p_t\right)p_{tt} + (1-3p^2)p_tp_{tt} \\
&\leq -\frac{\alpha\delta}{2}p_{tt}^2 + \frac{1}{\alpha\delta}\left(2\mu^2\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2(x,y,t)dxdy + \left(4 + 16\mu\delta\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\tilde{\eta}_1(x,y,0^+)dxdy\right)p_t^2\right).
\end{aligned} \tag{2.58}$$

The former follows from multiplying (2.54) by p_t and the latter from multiplying (2.54) by p_{tt}. Moreover, if we let

$$\beta_2 = \left(1 + \mu + 2^{3/2}\mu^{1/2}\delta^{1/2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\tilde{\eta}_1(x,y,0^+)dxdy\right), \tag{2.59}$$

$$\beta_3 = 4 + 2\mu^2 + 16\mu\delta \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \tilde{\eta}_1(x, y, 0^+) dxdy, \tag{2.60}$$

$$\tilde{\eta}_2 = \tilde{\eta}_1 + \frac{\alpha^2 \delta}{8\beta_2} p_t^2 = \frac{\mu T_0^2}{2\delta} + \frac{\lambda^2 \delta}{2} | \bigtriangledown p|^2 + \frac{(1-p^2)^2}{4\delta} + \frac{\alpha^2 \delta}{8\beta_2} p_t^2, \tag{2.61}$$

$$\tilde{\boldsymbol{q}}_2 = \tilde{\boldsymbol{q}}_1 + \frac{\alpha \lambda^2 \delta^2}{4\beta_2} p_t \bigtriangledown p_t = \lambda^2 \delta p_t \bigtriangledown p + \frac{\alpha \lambda^2 \delta^2}{4\beta_2} p_t \bigtriangledown p_t, \tag{2.62}$$

$$\begin{aligned} \tilde{G}_2 = \tilde{G}_1 &+ \frac{\alpha}{4\beta_2} \left(1 + \frac{\mu}{2} + 2^{3/2} \mu^{1/2} \delta^{1/2} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \tilde{\eta}_1(x, y, 0^+) dxdy \right) p_t^2 \\ &+ \frac{\alpha\mu}{8\beta_2} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} p_t^2(x, y, t) dxdy - \frac{\alpha \lambda^2 \delta^2}{4\beta_2} | \bigtriangledown p_t|^2, \end{aligned} \tag{2.63}$$

$$\tilde{\eta}_3 = \tilde{\eta}_2 + \frac{\alpha^2 \lambda^2 \delta^3}{8\beta_3} | \bigtriangledown p_t|^2 = \frac{\mu T_0^2}{2\delta} + \frac{\lambda^2 \delta}{2} | \bigtriangledown p|^2 + \frac{(1-p^2)}{4\delta} + \frac{\alpha^2 \delta}{8\beta_2} p_t^2 + \frac{\alpha^2 \lambda^2 \delta^3}{8\beta_3} | \bigtriangledown p_t^2| \tag{2.64}$$

$$\tilde{\boldsymbol{q}}_3 = \tilde{\boldsymbol{q}}_2 + \frac{\alpha^2 \lambda^2 \delta^3}{4\beta_3} p_{tt} \bigtriangledown p_t = \lambda^2 \delta p_t \bigtriangledown p + \frac{\alpha \lambda^2 \delta^2}{4\beta_2} p_t \bigtriangledown p_t + \frac{\alpha^2 \lambda^2 \delta^3}{4\beta_3} p_{tt} \bigtriangledown p_t, \tag{2.65}$$

and

$$\begin{aligned} \tilde{G}_3 = \tilde{G}_2 &+ \frac{\alpha}{4\beta_3} \left(4 + 16\mu\delta \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \tilde{\eta}_1(x, y, 0^+) dxdy \right) p_t^2 \\ &+ \frac{\alpha}{2\beta_3} \mu^2 \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} p_t^2(x, y, t) dxdy - \frac{\alpha^2 \delta^2}{8\beta_3} p_{tt}^2 \end{aligned} \tag{2.66}$$

we obtain the inequalities

$$\frac{\partial \tilde{\eta}_2}{\partial t} - \text{div } \tilde{\boldsymbol{q}}_2 \leq \tilde{G}_2 \text{ and } \frac{\partial \tilde{\eta}_3}{\partial t} = \text{div} \tilde{\boldsymbol{q}}_3 \leq \tilde{G}_3 \tag{2.67}$$

and these imply

$$
\begin{aligned}
&\frac{d}{dt}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(\frac{\mu T_0^2}{2\delta}+\frac{\lambda^2\delta|\bigtriangledown p|^2}{2}+\frac{(1-p^2)^2}{4\delta}+\frac{\alpha^2\delta}{8\beta_2}p_t^2\right)(x,y,t)dxdy\\
&\le -\frac{3\alpha}{4}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2(x,y,t)dxdy-\frac{\alpha\lambda^2\delta^2}{4\beta_2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p_t|^2(x,y,t)dxdy,
\end{aligned}
\tag{2.68}
$$

and

$$
\begin{aligned}
&\frac{d}{dt}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}\left(\frac{\mu T_0^2}{2\delta}+\frac{\lambda^2\delta|\bigtriangledown p|^2}{2}+\frac{(1-p^2)^2}{4\delta}+\frac{\alpha\delta}{8\beta_2}p_t^2+\frac{\alpha^2\lambda^2\delta^3}{8\beta_3}|\bigtriangledown p_t|^2\right)(x,y,t)dxdy\\
&\le -\frac{\alpha}{2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_t^2(x,y,t)-\frac{\alpha\lambda^2\delta^2}{4\beta_2}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}|\bigtriangledown p_t|^2(x,y,t)dxdy\\
&-\frac{\alpha^2\delta^2}{4\beta_3}\int_{-1/2}^{1/2}\int_{-1/2}^{1/2}p_{tt}^2(x,y,t)dxdy.
\end{aligned}
\tag{2.69}
$$

We leave it to the reader to supply the precise conclusions derivable from the inequalities (2.53), (2.63), and (2.69). The key point of these inequalities is that the parameter δ appears optimally.

3 Computational Experiments

In this section we present some numerical simulations of the system (2.2) - (2.4). We let N be an integer and set

$$
dx = dy = 1/N. \tag{3.1}
$$

Our approximate solutions will be constant on the cells

$$
\Omega_{i,j}=\left\{(x,y)\middle|-\frac{1}{2}+\frac{(i-1)}{N}<x<-\frac{1}{2}+\frac{i}{N}\text{ and }-\frac{1}{2}+\frac{(j-1)}{N}<y<-\frac{1}{2}+\frac{j}{N}\right\} \tag{3.2}
$$

where $1\le i,j\le N$ and thus the cell averages $(T_{i,j},p_{i,j})$ may also be thought of as the point values at the cell centers

$$
(x_i,y_j)=\left(-\frac{1}{2}+\frac{2i-1}{2N},\ -\frac{1}{2}+\frac{2j-1}{2N}\right). \tag{3.3}
$$

We impose the boundary conditions

$$\frac{\partial T}{\partial n} = \frac{\partial p}{\partial n} = 0 \quad , \quad (x, y) \in \partial\Omega \tag{3.4}$$

by insisting that the extended grid functions satisfy

$$\left.\begin{aligned} &(T_{0,k}, p_{0,k}) = (T_{1,k}, p_{1,k}) \,, \\ &(T_{N+1,k}, p_{N+1,k}) = (T_{N,k}, p_{N,k}) \,, \\ &(T_{k,0}, p_{k,0}) = (T_{k,1}, p_{k,1}) \,, \\ \text{and} \\ &(T_{k,N+1}, p_{k,N+1}) = (T_{k,N}, p_{k,N}) \end{aligned}\right\} \tag{3.5}$$

for $1 \leq k \leq N$.

For any function u defined on the grid and satisfying (3.5) we let

$$\Delta_N u_{i,j} = N^2 \left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} \right) \tag{3.6}$$

be the discrete Laplacian applied to u. For functions u and v satisfying (3.5) we define

$$[u, v] = \sum_{i,j=1}^{N} u_{i,j} v_{i,j} / N^2 \tag{3.7}$$

and note that

$$-[u, \Delta_N u] = \sum_{i=1}^{N} \sum_{j=1}^{N-1} \left(u_{i,j+1} - u_{i,j} \right)^2 + \sum_{j=1}^{N} \sum_{i=1}^{N-1} \left(u_{i+1,j} - u_{i,j} \right)^2 . \tag{3.8}$$

Such grid functions also satisfy the discrete version of Lemma 1, namely the inequality

$$[u^2, u^2] = [u^4, 1] \leq 4 \left(\frac{(1+\epsilon)}{\epsilon} [u, u] - \epsilon [u, \Delta_N u] \right)^2 \tag{3.9}$$

for every $\epsilon > 0$.

Finally, we replace (2.2) - (2.4) by the system

$$\dot{T}_{i,j} + (1 - p_{i,j}^2) \dot{p}_{i,j} - a^2 \Delta_N T_{i,j} = 0 \tag{3.10}$$

and

$$\alpha\delta\dot{p}_{i,j} - \lambda^2\delta^2\Delta_N p_{i,j} = (\mu T_{i,j} + p_{i,j})(1 - p_{i,j}^2) \tag{3.11}$$

where $T_{i,j}$ and $p_{i,j}$ satisfy the discrete boundary conditions (3.5) and the symbol $\cdot$ denotes differentiation with respect to t. Solutions of (3.10) and (3.11) obey the pointwise estimate that if $-1 \le p_{i,j}(0^+) \le 1,\ 1 \le i,j \le N$, then $-1 \le p_{i,j}(t) \le 1,\ 1 \le i,j \le N$ for all $t > 0$. This system also satisfies estimates which are the exact analogue of those obtained in section (2). Corresponding to (2.8) we have the identity

$$[T + p - p^3/3, 1](t) \equiv h_0 \tag{3.12}$$

while the analogues of (2.11) and (2.15) are the inequalities

$$\frac{d}{dt}\left(\left[\left(\frac{\mu T^2}{2\delta} + \frac{(1-p^2)^2}{4\delta}\right), 1\right] - \frac{\lambda^2\delta}{2}[p, \Delta_N p]\right)(t) = -\alpha[p_t, p_t](t) + \frac{\mu a^2}{\delta}[T, \Delta_N T](t), \tag{3.13}$$

and

$$\begin{aligned} &\frac{d}{dt}\left(\left[\frac{\mu T^2}{2\delta} + \frac{(1-p^2)^2}{4\delta}, 1\right] - \frac{\lambda^2\delta}{2}[p, \Delta_N p] - \frac{\alpha a^2}{2}[T, \Delta_N T]\right)(t) \\ &\le -\frac{\alpha}{2}\left([p_t, p_t] + [T_t, T_t]\right)(t) + \frac{\mu a^2}{\delta}[T, \Delta_N T](t). \end{aligned} \tag{3.14}$$

We spare the reader the detailed analogues of (2.39), (2.41), and (2.45). Suffice it to say if we replace terms like $\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} f(x,y,t)dxdy$ by $[f,1](t)$ and terms like $\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} \mid \nabla f \mid^2 (x,y,t)dxdy$ by $-[f, \Delta_N f](t)$, then the resulting inequalities go through intact.

When doing simulations with the discrete system (3.10) and (3.11) we link the small parameter δ to the grid $dx = dy = 1/N$; specifically we set

$$\delta = 1/N \tag{3.15}$$

and restrict our attention to initial data satisfying

$$N\left[\frac{\mu T^2}{2} + \frac{(1-p^2)^2}{4}, 1\right](0^+) - \frac{\lambda^2}{2N}[p, \Delta_N p](0^+) - \frac{\alpha a^2}{2}[T, \Delta_N T](0^+) = O(1). \tag{3.16}$$

Interesting data satisfying (3.16) may be achieved in a variety of ways. Below we outline one such construction. We let Γ be a simple closed curve of finite arclength $L(\Gamma)$ which is wholly contained in

Ω, $\mathcal{S}_c$ be all cells $\Omega_{i,j}$ which are cut by Γ, $\mathcal{S}_I$ be all cells $\Omega_{i,j}$ which are interior to the region surrounded by Γ, and $\mathcal{S}_E$ be those cells $\Omega_{i,j}$ which are in Ω and exterior to Γ. For definiteness we choose

$$p_{i,j}(0^+) = \begin{cases} 1, & \text{if } \Omega_{i,j} \in \mathcal{S}_E \\ p^*_{i,j} \in [-1,1]\,, & \text{if } \Omega_{i,j} \in \mathcal{S}_c \\ -1, & \text{if } \Omega_{i,j} \in \mathcal{S}_I \end{cases} \tag{3.17}$$

and

$$T_{i,j}\left(0^+\right) = h_0 - \left[\left(p - p^3/3\right)\left(0^+\right), 1\right] = O\left(1/N^{1/2}\right). \tag{3.18}$$

Such data models the situation where initially water surrounds ice. With such data it is easily checked that $N\left[T^2\left(0^+\right), 1\right] = P(1)$, while $N\left[(1-p^2)^2, 1\right]$ and $-\frac{1}{N}\left[p, \Delta_N p\right]$ are $O(L(\Gamma))$ and thus the functional defined in (3.16) is $O(1)$ independently of N. For such data we note that $\delta^3\left[\Delta_N p, \Delta_N p\right] = \frac{1}{N^3}\left[\Delta_N p, \Delta_N p\right]$ is also $O(L(\Gamma))$ independently of N. The last functional enters in the discrete analogue of (2.68).

The simulations we present were all run with the following parameters:

$$(\alpha, \lambda, a, \mu) = (1,1,1,1)\,. \tag{3.19}$$

We chose $N = 200$

$$dx = dy = \delta = 1/200 \tag{3.20}$$

and

$$dt = dx/10. \tag{3.21}$$

With these parameters

$$m1 \overset{def}{=} dt/(dx)^2 = 10 \tag{3.22}$$

and

$$m2 \overset{def}{=} \frac{\delta dt}{(dx)^2} = \frac{1}{10} \tag{3.23}$$

and thus we were compelled to use an implicit integration scheme for (3.10). Our choice was ADI working with the fixed tri-diagonal matrix whose non-zero entries are

$$A(i,i) = \begin{cases} 1 + m1 & \text{if } i = 1 \text{ and } i = 200 \\ 1 + 2m1 & \text{if } 2 \le i \le 199 \end{cases} \tag{3.24}$$

and

$$A(i,i+1) = A(i+1,i) = -m1, \quad 1 \le i \le 199. \tag{3.25}$$

We used a first order explicit Euler scheme on (3.11).

Our first simulation was run with the following choice of initial data:

$$p_{i,j}(0^+) = \begin{cases} 1, \text{ if } \begin{array}{lll} \{101+i \le j \le 200 & \text{and} & 1 \le i \le 99\} \text{ or} \\ \{302-i \le j \le 200 & \text{and} & 102 \le i \le 200\} \text{ or} \\ \{1 \le j \le 100-i & \text{and} & 1 \le i \le 99\} \text{ or} \\ \{1 \le j \le -101+i & \text{and} & 102 \le i \le 200\}, \end{array} \\ \\ 0, \text{ if } \begin{array}{lll} \{100+i = j & \text{and} & 1 \le i \le 100\} \text{ or} \\ \{301-i = j & \text{and} & 101 \le i \le 200\} \text{ or} \\ \{101-i = j & \text{and} & 1 \le i \le 100\} \text{ or} \\ \{-100+i = j & \text{and} & 101 \le i \le 200\}, \end{array} \\ \\ -1, \text{ if } \begin{array}{lll} \{102-i \le j \le 99+i & \text{and} & 2 \le i \le 100\} \text{ or} \\ \{-99+i \le j \le 300-i & \text{and} & 101 \le i \le 199\}. \end{array} \end{cases} \tag{3.26}$$

This data satisfies $[p,1] = [p^3,1] = 0$. We chose $h_0 = .05$ and $T_{i,j}(0^+) \equiv .05, \ 1 \le i,j \le 200$.

The initially superheated square block of ice converged to a circular block centered at $(0,0)$ with a radius consistent with the $\delta = 0^+$ asymptotics. Specifically, if we grant that the "equilibrium" curve separating the ice from the water is a circle of radius R, then the "Gibbs-Thomson" relation (1.6), with our choice of parameters, implies that

$$\frac{.005}{2^{1/2}R} = -T_M \tag{3.27}$$

while (3.12) implies that

$$T_M = .05 - [p - p^3/3, 1]. \tag{3.28}$$

Noting that $p_{i,j} \simeq -1$ inside of the circle and $p_{i,j} \simeq +1$ outside yields

$$[p - p^3/3, 1] = \frac{2}{3}\left(1 - 2\pi R^2\right) \tag{3.29}$$

and (3.27)-(3.29) imply that R satisfies

$$\frac{4\pi}{3}R^2 + \frac{.005}{2^{1/2}R} = \frac{2}{3} - .05. \tag{3.30}$$

(3.30) has one positive solution close to zero and a second larger solution $R = .3808$ which is the approximate equilibrium radius we obtain in our simulation. This radius, when substituted into the Gibbs-Thomson relation (3.27) yields a melt temperature consistent with what we observe. The results of this simulation are shown in Figure 1.

Our final simulation starts with 16 regularly spaced circular blocks of ice surrounded by water. Specifically

$$p_{i,j}(0^+) = \begin{cases} -1, \text{ if } & \sqrt{(i-40m)^2+(j-40n)^2} \le 15 \\ & \text{and } 1 \le m,n \le 4 \\ 1, & \text{otherwise.} \end{cases} \tag{3.31}$$

For this data

$$[(p - p^3/3)(0^+), 1] = .2885. \tag{3.32}$$

We again chose h_0 to be .05 and at $t = 0$ took the uniform temperature field

$$T_{i,j}(0^+) = h_0 - [(p - p^3/3)(0^+), 1] = -.2385. \tag{3.33}$$

The solutions using this initial data converged to the same equilibrium as before but the approach was far more interesting. The solutions at times $t = .05,\ .17,\ .24,\ .4,\ .6,\ .7,\ 2, 3.3$, and 12.5 are shown in Figures 2-10.

We also ran both sets of data with the "intermediate" model and obtained virtually identical results.

Explanation of Graphics

In Figures 1-10 the upper left frame is a contour plot of p and p is 1 in a neighborhood of the boundaries $x = \pm 1/2$ and $y = \pm 1/2$ and the upper right hand frame is a contour plot of T. In Figure 1 the lower left plot shows p, T and $p - p^3/3 + T$ along the lines $x = 0,\ y = 0$, and the 45^o diagonal through the origin. These plots overlay one another because of the circular symmetry of the final state. In Figure 1 the bottom right plot again displays the same information. In Figures 2-10 the bottom left plot shows p, T, and $p - p^3/3 + T$ along the 45^o diagonal through the origin and the bottom right plot shows the same quantities on the line $x = 0$. The reader interested in seeing a movie of the second simulation should consult reference 3 on the author's web site: http://www.math.cmu.edu/math/people/greenberg.html.

4 Concluding Remarks

We have established the existence of properly scaled entropies of successively higher order in the space and time derivatives of T and p which are bounded on solutions of (1.1) and (1.2). These entropies yield information (i) about the sharp-interface, $\delta = 0^+$ limits of solutions of (1.1) and (1.2) and (ii) large t information about the solutions of (1.1) and (1.2) at fixed δ. More importantly we have shown correspondingly spatially discrete entropies for the spatially discretized version of this system which are faithful to the entropies of the continuous system.

We have carried out the calculations to verify that the system (1.4) and (1.5) with $m = 0$, which has been studied extensively by Caginalp [5-7], is endowed with similar entropies. As noted earlier, this system is not endowed with the pointwise estimates $-1 \leq p(x, y, t) \leq 1$, but the fact that the temperature difference, T, appears linearly in (1.5) saves the day. We have not succeeded in carrying out our program of rigorous estimates for (1.4) and (1.5) when $n = m \geq 2$.

Perhaps the most important /interesting conclusion of this study is that under mild and natural conditions on the initial data the solutions of (1.1) and (1.2) satisfying $\frac{\partial T}{\partial n} = \frac{\partial p}{\partial n} = 0$ on $\partial\Omega$ asymptotically evolve as solutions of the reduced system (1.10), (1.11), and (1.13).

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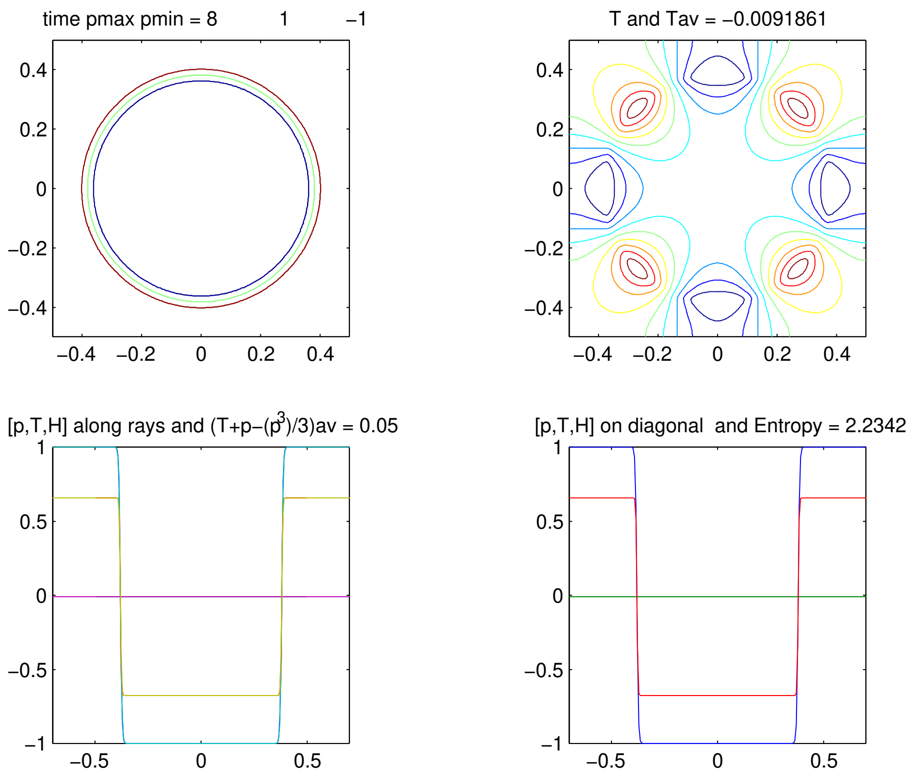
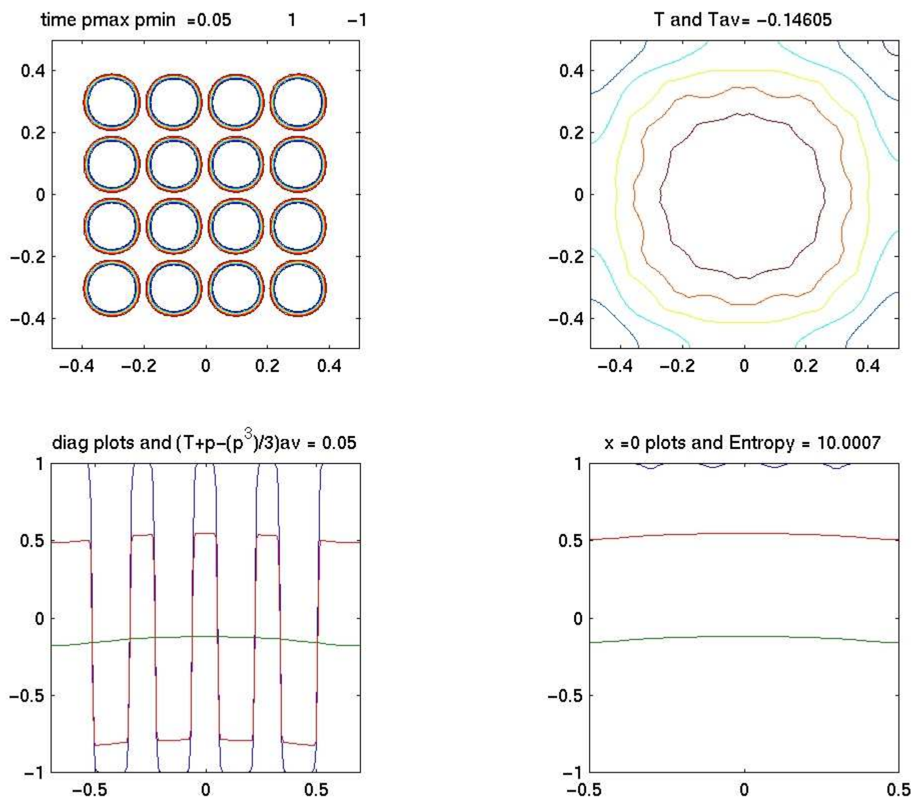


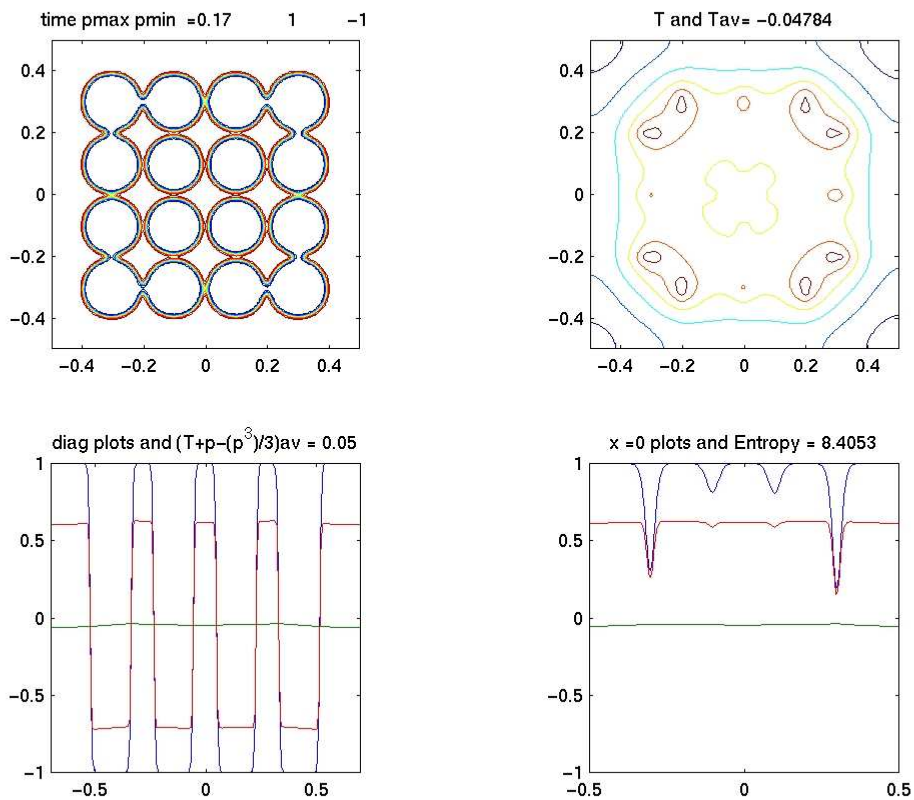
time pmax pmin = 8 1 −1
T and Tav = −0.0091861
[p,T,H] along rays and (T+p−(p3)/3)av = 0.05
[p,T,H] on diagonal and Entropy = 2.2342

Figure 1



time pmax pmin =0.05 1 −1
T and Tav= −0.14605
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 10.0007

Figure 2



time pmax pmin =0.17 1 −1
T and Tav= −0.04784
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 8.4053

Figure 3

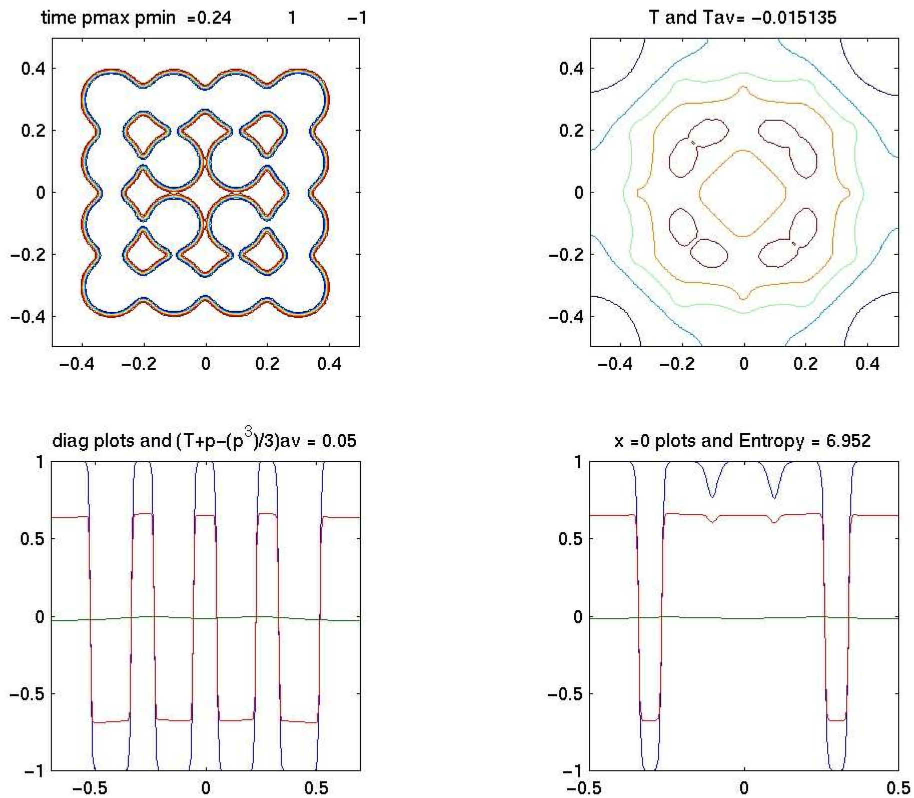
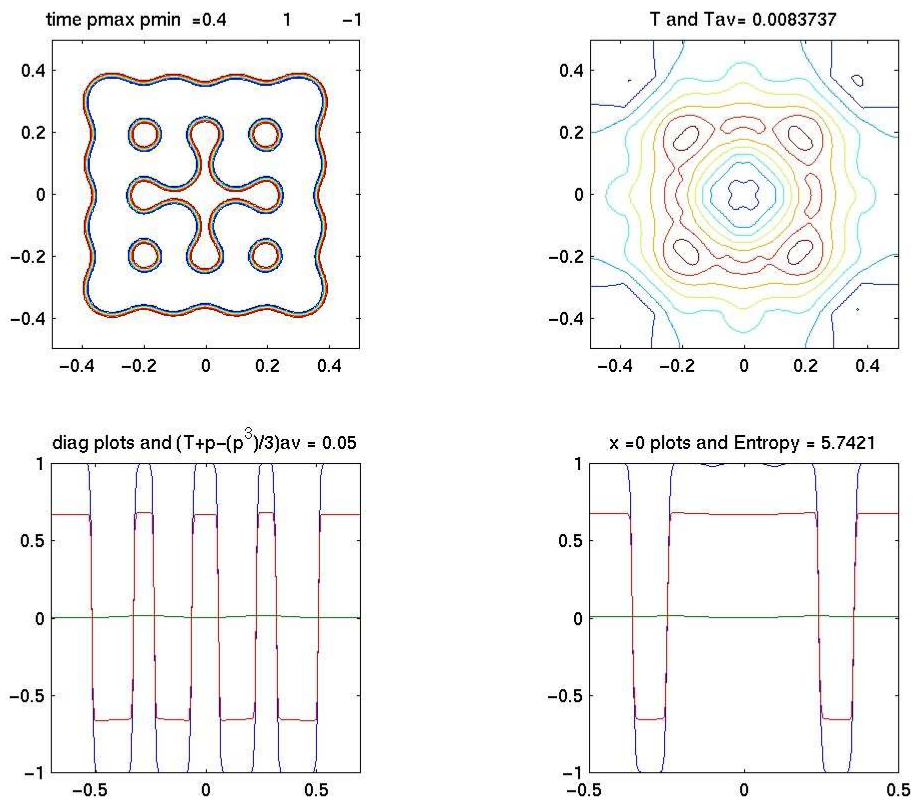

time pmax pmin =0.24 1 −1
T and Tav= −0.015135
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 6.952

Figure 4



time pmax pmin =0.4 1 −1
T and Tav= 0.0083737
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 5.7421

Figure 5

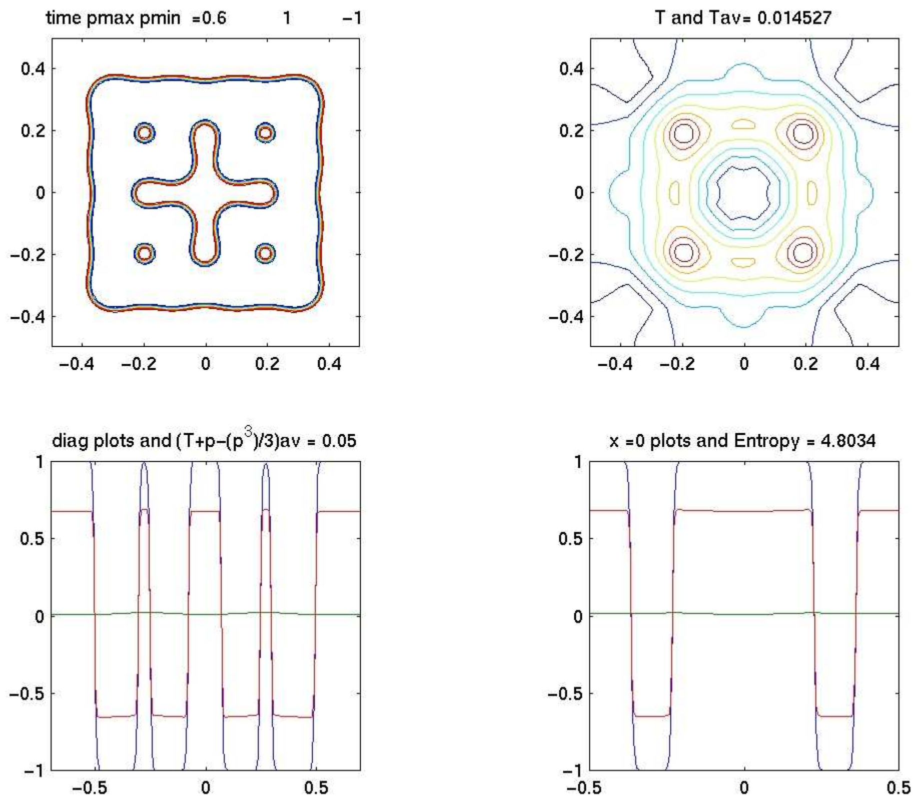

time pmax pmin =0.6 1 −1
T and Tav= 0.014527
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 4.8034

Figure 6

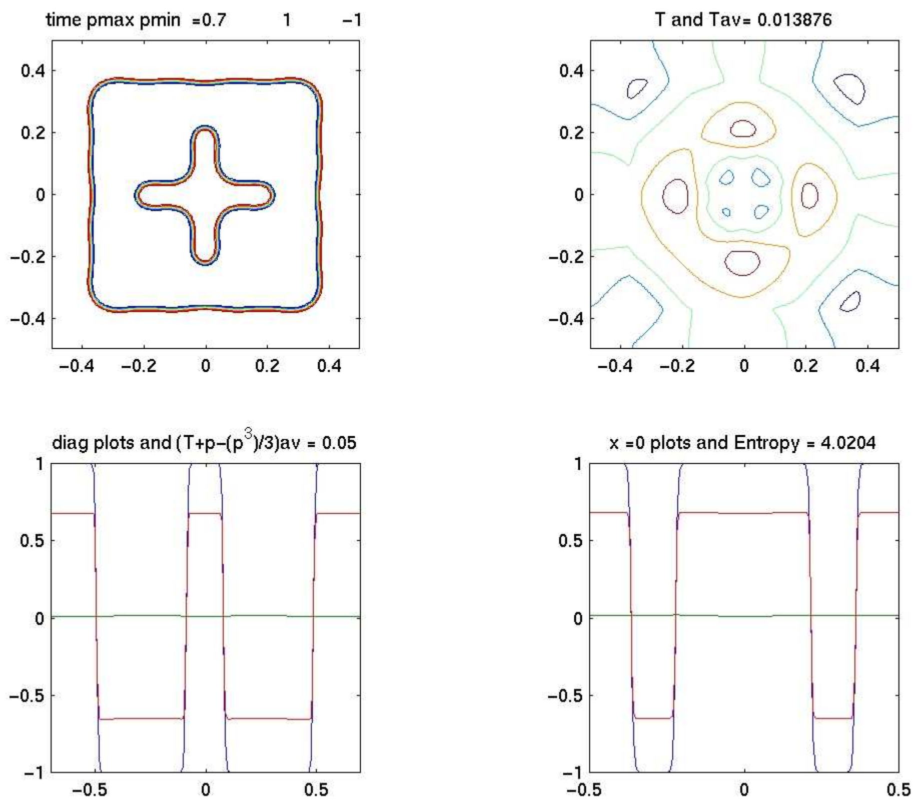
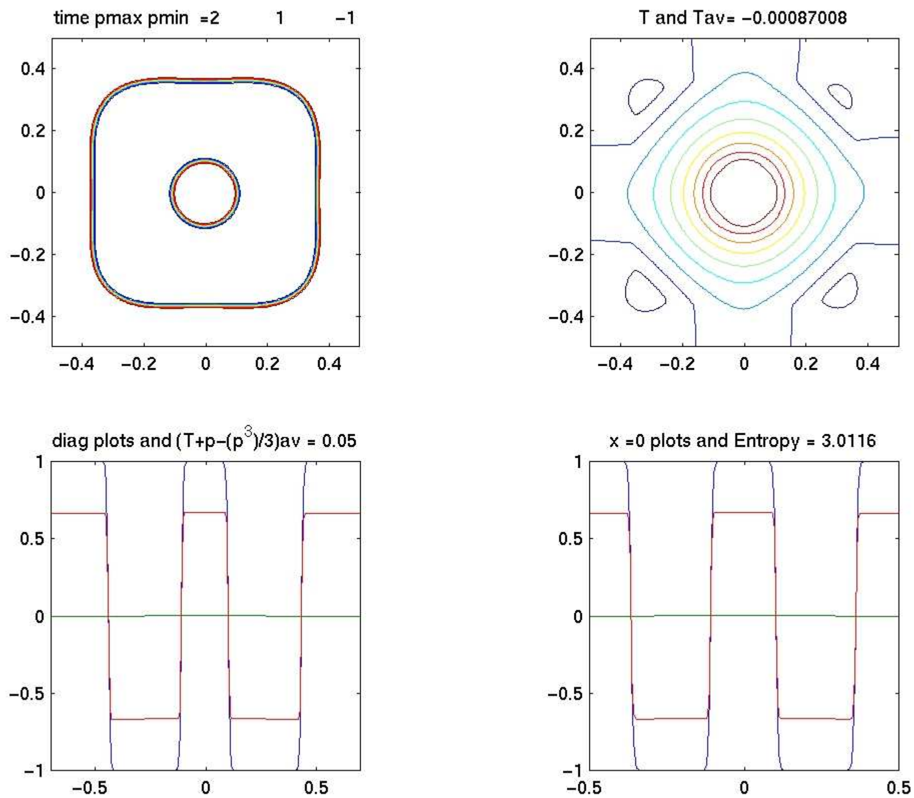

time pmax pmin =0.7 1 −1
T and Tav= 0.013876
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 4.0204

Figure 7



time pmax pmin =2 1 −1
T and Tav= −0.00087008
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 3.0116

Figure 8

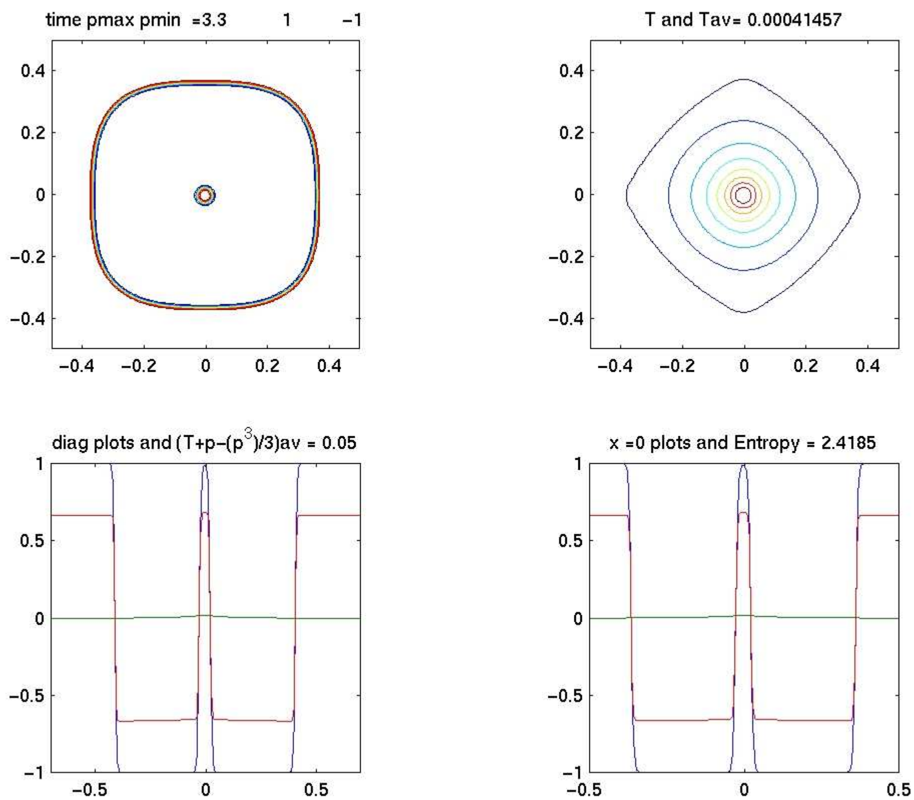

time pmax pmin =3.3 1 −1
T and Tav= 0.00041457
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 2.4185

Figure 9

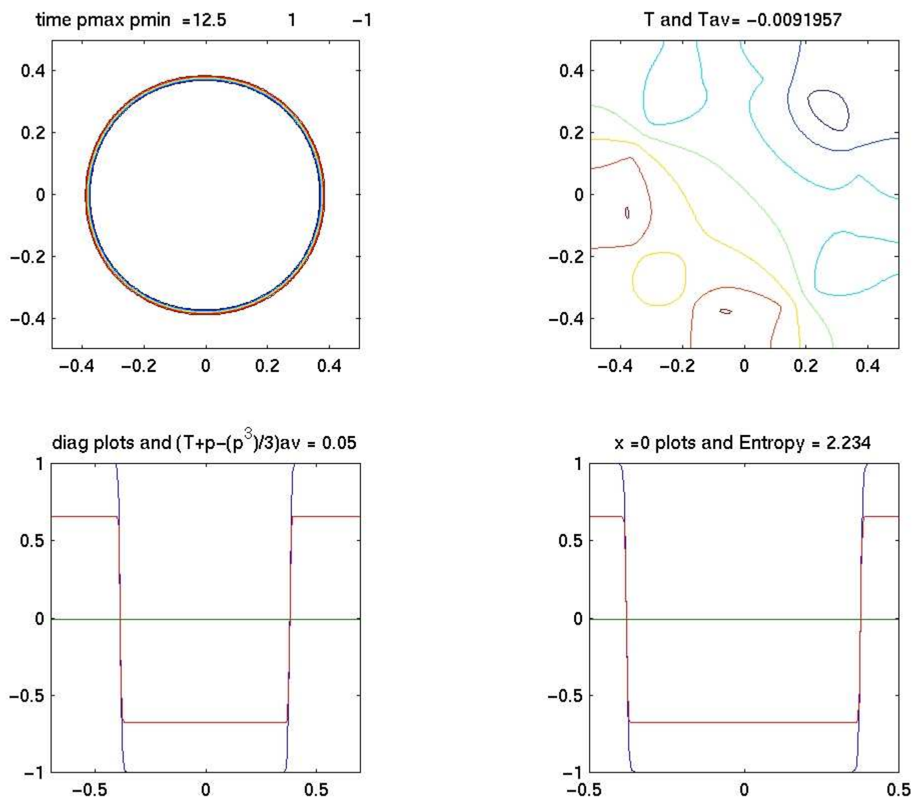

time pmax pmin =12.5 1 −1
T and Tav= −0.0091957
diag plots and (T+p−(p^3)/3)av = 0.05
x =0 plots and Entropy = 2.234

Figure 10