

## RAPIDLY CONVERGING PHASE FIELD MODELS VIA SECOND ORDER ASYMPTOTICS

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**Abstract.** We consider phase field models with the objective of approximating sharp interface models. By using second order asymptotics in the interface thickness parameter,  $\varepsilon$ , we develop models in which the order  $\varepsilon$  term is eliminated, suggesting more rapid convergence to the  $\varepsilon = 0$  (sharp interface) limit. In addition we use non-smooth potentials with a non-zero gradient at the roots. These changes result in an error that is 1/200 of the classical models in sample one-dimensional calculations. Alternatively, one can use 1/100 of the node points in each direction for our proposed models and still obtain the same accuracy as one would with the classical model. We expect that this will greatly facilitate two and three dimensional calculations of dendritic growth with physically realistic parameters.

**1. Introduction.** Phase field models nowadays belong to the established techniques for the description and numerical simulation of phase transitions, see references in [4]. The model is based on the assumption of a diffuse phase transition layer of usually very small thickness, that encompasses the transition between the two pure phases. Phase field models can be interpreted and applied with two different aims: the first is a physically more accurate description of the phase transition than by the sharp interphase model, the second is the approximation of a sharp interface model by a model of simpler mathematical structure, which is also easier to implement in a numerical algorithm. From the point of view of numerical simulation, the second motivation is considerably more important, because the physically realistic width of the diffuse phase transition layer of around  $10^{-8}$  is usually not resolved by any computational grid, even in adaptive computations. The desired sharp interface limit can be attained through a spectrum of phase field models. Therefore it may be advantageous to use this freedom in order to construct a model for which the numerical scheme is likely to better approximate the sharp interface model for

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a given  $\varepsilon$ . This topic shall be studied in the present article for phase transitions between two states, e.g. liquid or solid, in pure material. We use a phase field model of the type [4]:

$$\alpha\varepsilon^2\partial_t\varphi - \varepsilon^2\Delta\varphi + f'(\varphi) - \frac{\varepsilon}{\sigma}g'(\varphi)u = 0, \text{ and} \tag{1}$$

$$\partial_t(u + \frac{l}{2}\varphi) = \nabla \cdot (K\nabla u). \tag{2}$$

Here,  $\varphi$  is the phase field, with  $\varphi = 1$  for liquid and  $\varphi = -1$  for solid material,  $u$  is the dimensionless temperature,  $\varepsilon$  is the approximation parameter roughly representing the width of the diffuse phase transition layer,  $\alpha$  is the kinetic coefficient,  $\sigma$  the surface tension, divided by the entropy difference between phases (often called the capillary length,  $d_0$ ),  $f$  is a double well or double obstacle potential,  $g$  is a further constitutive function,  $l$  is the latent heat and  $K$  the heat diffusivity (see [4] for complete dimensions). For a suitable — but not uniquely defined — choice of  $f$  and  $g$  the solutions of the model converge for  $\varepsilon \rightarrow 0$  to the solutions of the sharp interface problem with curvature- and kinetic undercooling,

$$\partial_t u = \nabla \cdot (K\nabla u) \text{ in } \Omega_\ell(t) \cup \Omega_s(t), \tag{3}$$

$$[K\nabla u \cdot n]_-^+ = -lv \text{ and} \tag{4}$$

$$u = -\sigma(\alpha v + \kappa) \text{ on } \Gamma_I(t). \tag{5}$$

Here,  $\Omega_\ell(t)$  and  $\Omega_s(t)$  denote the liquid and solid domain,  $\Gamma_I(t)$  the phase interphase,  $n$  the normal vector of the interface, directed to the exterior of the solid domain,  $v$  the velocity of the solid-liquid interphase,  $\kappa$  the curvature, and  $[K\nabla u \cdot n]$  the jump in the heat flux at the interface. The “original” choices for the functions  $f$  and  $g$  are  $f(\varphi) = \frac{1}{2}(\varphi^2 - 1)^2$  and  $g(\varphi) = \frac{2}{3}\varphi$ , but many authors have proposed alternative constitutive functions. Often the double well potential is replaced by a double obstacle potential [2], [6], whose advantage is that the phase field actually attains its pure phase values of  $\varphi = +1$  and  $\varphi = -1$  in most of the computational domain (and not merely approximates it), and in even more applications the function  $g$  is chosen such that the minima of the combined potential  $\varphi \mapsto f(\varphi) - \frac{\varepsilon}{\sigma}g(\varphi)u$  are kept at  $\varphi = \pm 1$ , which is not the case for  $g(\varphi) \sim \varphi$ . The aim of this article is a more systematical study of the appropriate choice of  $f$  and  $g$ , potentially leading to a model that is more efficient for a given  $\varepsilon$  when the surface tension is very small. We accomplish this by reexamining the asymptotic analysis that establishes the connection between phase field and sharp interface problems and choosing  $f$  and  $g$  so that the first order corrector term in the asymptotic expansion cancels. The spirit is the same as adopted by Almgren [1], but, as we will see, a suitable choice of the functions at a certain step of our approach yields a more accurate interface condition for non-zero interface thickness.

**2. Optimizing through asymptotic expansion.** We briefly recall the well-known matched asymptotic expansion of the phase field model. This expansion consists of two parts, an outer expansion valid far away from the actual solid-liquid interface, and an inner expansion valid close to the interface. The outer expansion is given in cartesian coordinates by

$$\psi_\varepsilon(t, x) = \psi_0(t, x) + \varepsilon\psi_1(t, x) + \varepsilon^2\psi_2(t, x) + \dots \text{ for } \psi = u, \varphi. \tag{6}$$

The coefficients  $\psi_j$  in this expansion shall be bounded functions. They may have a discontinuity at the interface  $x \in \Gamma(t)$  but are smooth otherwise. For the inner expansion we use local coordinates chosen in a neighbourhood of the curve (or

surface in three dimensions)  $\Gamma = \Gamma_\varepsilon(t)$  of zeros of the phase field  $\varphi$ , evaluated at time  $t$ . This curve depends on the chosen phase field parameter  $\varepsilon$ ; this fact is indicated by the index  $\varepsilon$ . To a point  $x \in \Omega$ , let  $r_\varepsilon(t, x)$  denote the signed distance of  $x$  to  $\Gamma_\varepsilon(t)$  (with positive  $r_\varepsilon(t, x)$  for  $x$  in the liquid domain), and let  $(r_\varepsilon, s_\varepsilon)$  denote a local orthogonal coordinate system near  $\Gamma_\varepsilon(t)$ . For simplicity of the notation we skip the subscript  $\varepsilon$  in the sequel. The local coordinates satisfy

$$\begin{aligned} |\nabla r|^2 &= 1, \quad \nabla r \cdot \nabla s_i = 0 \text{ for } i = 1, \dots, N, \\ \partial_t r(t, x) &= -v, \\ \Delta r &= \frac{\kappa + 2\Pi r}{1 + \kappa r + \Pi r^2}. \end{aligned}$$

Here  $\kappa$  and  $\Pi$  denote the mean and Gaussian curvatures,  $N$  is the space dimension and the subscript  $i$  refers to the corresponding component of a  $N$ -dimensional vector. For the corresponding transform of a function  $u$ ,

$$u(t, x) = \tilde{U}(t, r(t, x), s(t, x)),$$

the differential operators transform according to

$$\begin{aligned} \partial_t u &= (\partial_t + \partial_t r \partial_r + \partial_t s \cdot \partial_s) \tilde{U} \quad \text{and} \\ \Delta u &= (\Delta r \partial_r + \Delta s \cdot \partial_s + \partial_r^2 + |\nabla s|^2 \partial_s^2) \tilde{U}. \end{aligned}$$

In the inner expansion, the solution of the phase field model is represented first in the new variables  $t, r, s$  and then in  $\varrho = r/\varepsilon$  and expanded in series of powers of  $\varepsilon$ ,

$$\Psi_\varepsilon(t, \varrho, s) = \Psi_0(t, \varrho, s) + \varepsilon \Psi_1(t, \varrho, s) + \varepsilon^2 \Psi_2(t, \varrho, s) + \dots \text{ for } \varphi = \Phi, U. \quad (7)$$

The equations are also expanded in orders of  $\varepsilon$ , and a comparison of the coefficients with respect to different orders of  $\varepsilon$  for both the inner and outer expansions is done. The asymptotic expansions of the differential operators are

$$\begin{aligned} \partial_t &\sim \varepsilon^{-1} \partial_t r \partial_\varrho + (\partial_t + \partial_t s \partial_s) \quad \text{and} \\ \Delta &\sim \varepsilon^{-2} \partial_\varrho^2 + \varepsilon^{-1} \Delta r \partial_\varrho + (\Delta s \cdot \partial_s + |\nabla s|^2 \partial_s^2). \end{aligned}$$

In an intermediate region of distance proportional to  $\sqrt{\varepsilon}$  the inner and outer expansions describe the same function. This is realized via matching conditions for both expansions. They can be formulated after writing the outer expansion in terms of the local variables. From the representation  $\varrho = \frac{x - y_\varepsilon(t)}{\varepsilon}$  follows

$$\Psi_\varepsilon(t, \varrho) = \psi_\varepsilon(t, y_\varepsilon(t) + \varepsilon \varrho).$$

This condition is valid for large  $\varrho$  or  $-\varrho$ . The matching is done with the help of the expansions (6), (7) and a corresponding expansion of  $y_\varepsilon(t)$  [3],

$$y_\varepsilon(t) = y_0(t) + \varepsilon y_1(t) + \dots \quad (8)$$

The combination of this expansion with the outer expansion (6) leads to

$$\begin{aligned} \psi_\varepsilon(t, y_\varepsilon(t) + \varepsilon \varrho) &= \psi_0(t, y_0(t)_\pm) \\ &+ \varepsilon (\psi_1(t, y_0(t)_\pm) + \partial_n \psi_0(t, y_0(t)_\pm) (y_1(t) + \varrho)) + \dots \end{aligned} \quad (9)$$

Here the index  $\pm$  at  $y_0(t)$  indicates the limit at the interface from the right (for  $\varrho > 0$ ) or left (for  $\varrho < 0$ ); it is necessary since the coefficient functions  $\psi_k$  may be discontinuous there. This leads to the matching conditions of order  $\varepsilon^0$ ,

$$\lim_{\varrho \rightarrow \pm\infty} \Psi_0(t, \varrho) = \psi_0(t, y_0(t)_\pm) \quad (10)$$

and the corresponding condition for the  $O(\varepsilon)$  terms for large  $|\varrho|$

$$\Psi_1(t, \varrho) \sim \psi_1(t, y_0(t)_\pm) + (y_1(t) + \varrho)\partial_n u_0(t, y_0(t)_\pm). \quad (11)$$

After this short introduction to the technique of asymptotic expansions we formulate the main result:

**Proposition 1.** *Assume that the outer and inner expansions (6) and (7) are valid up to the order  $\varepsilon^2$  with bounded coefficient functions, and that the surface  $\Gamma_\varepsilon(t)$  converges for  $\varepsilon \rightarrow 0$  to a  $C^2$ -smooth interface  $\Gamma_0(t)$  for every  $t > 0$ . Then, for the choice (26) of the function  $g$ , the first order correction  $\Phi_1$  in the inner expansion vanishes, and the dynamical Gibbs-Thomson condition is satisfied through order  $\varepsilon$  in the asymptotic expansion in a suitable averaged sense described by relation (29) below.*

**Verification** From the outer expansion (6) and the differential equations we derive the following sequence of problems.

The  $O(1)$  problem:

$$\partial_t u_0 + \frac{1}{2}\partial_t \varphi_0 = \nabla \cdot (K\nabla u_0), \quad (12)$$

$$f'(\varphi_0) = 0. \quad (13)$$

From the second equation here follows  $\varphi_0 \in \{\pm 1\}$  almost everywhere in  $\Omega$ . Then the term  $\partial_t \varphi_0$  is a distribution whose support coincides with the set of discontinuities of  $\varphi_0$ .

The  $O(\varepsilon)$  problem:

$$\partial_t u_1 + \frac{1}{2}\partial_t \varphi_1 = \nabla \cdot (K\nabla u_1), \quad (14)$$

$$f''(\varphi_0)\varphi_1 - \frac{1}{\sigma}g'(\varphi_0)u_0 = 0. \quad (15)$$

The  $O(\varepsilon^2)$  problem:

$$\partial_t u_2 + \frac{1}{2}\partial_t \varphi_2 = \nabla \cdot (K\nabla u_2), \quad (16)$$

$$\begin{aligned} \alpha\partial_t \varphi_0 - \Delta \varphi_0 + \frac{1}{2}f'''(\varphi_0)\varphi_1^2 + f''(\varphi_0)\varphi_2 \\ - \frac{1}{\sigma}g''(\varphi_0)\varphi_1 u_0 - \frac{1}{\sigma}g'(\varphi_0)u_1 = 0. \end{aligned} \quad (17)$$

Here the Taylor expansions

$$f'(\varphi_\varepsilon) = f'(\varphi_0) + \varepsilon f''(\varphi_0)\varphi_1 + \varepsilon^2 \left(\frac{1}{2}f'''(\varphi_0)\varphi_1^2 + f''(\varphi_0)\varphi_2\right) + \dots$$

and an analogous expansion for  $g'(\varphi_\varepsilon)$  are employed.

The inner expansion follows from substitution of (7) into (1) and (2):

$$\begin{aligned} -\partial_\varrho^2 \Phi + f'(\Phi) + \varepsilon \left(-\frac{1}{\sigma}g'(\Phi)U - \Delta r \partial_\varrho \Phi + \alpha \partial_{tr} \partial_\varrho \Phi\right) \\ + \varepsilon^2 \left(\alpha \partial_t \Phi + \alpha \partial_{ts} \partial_s \Phi - |\nabla s|^2 \partial_s^2 \Phi - \Delta s \partial_s \Phi\right) = 0, \end{aligned} \quad (18)$$

$$\begin{aligned} K\partial_\varrho^2 U + \varepsilon \left(-\partial_{tr} \partial_\varrho U - \frac{1}{2} \partial_{tr} \partial_\varrho \Phi + K\Delta r \partial_\varrho U\right) \\ - \varepsilon^2 \left(\partial_t U + \partial_{ts} \partial_s U + \frac{1}{2} \partial_t \Phi + \frac{1}{2} \partial_{ts} \partial_s \Phi - K|\nabla s|^2 \partial_s^2 U - K\Delta s \partial_s U\right) = 0. \end{aligned} \quad (19)$$

The  $O(1)$  problem is

$$K\partial_\varrho^2 U_0 = 0, \quad (20)$$

$$-\partial_\varrho^2 \Phi_0 + f'(\Phi_0) = 0. \quad (21)$$

The first equation here implies that  $U_0$  is linear,  $U_0(\varrho) = A\varrho + B$ . From the matching condition to the outer solution we conclude  $A = 0$ , because  $\lim_{\varrho \rightarrow \pm\infty}$  is bounded. Hence  $U_0$  is independent of  $\varrho$ . The second equation is supplemented by the condition  $\Phi_0(0) = 0$  that follows from the choice of the coordinate system and by  $\lim_{\varrho \rightarrow \pm\infty} \Phi_0(\varrho) = \varphi_0(t, \Gamma_{\pm}) = \pm 1$ . The latter is the matching condition of order  $O(1)$ , with  $\varphi_0(t, \Gamma_{\pm})$  being the limit of  $\varphi_0$  on the interface from the liquid (for index  $+$ ) or solid (for index  $-$ ) side. The resulting problem has a unique solution  $\Phi_0(\varrho)$  that does not depend on  $s$  and  $t$ . In the case  $f(\Phi) = \frac{1}{2}(\Phi^2 - 1)^2$  this solution is given by  $\Phi_0(\varrho) = \tanh(\varrho)$ .

The  $O(\varepsilon)$  problem is

$$\begin{aligned} K\partial_{\varrho}^2 U_1 - \frac{1}{2}\partial_t r_0 \partial_{\varrho} \Phi_0 &= 0, \\ -\partial_{\varrho}^2 \Phi_1 + f''(\Phi_0)\Phi_1 - \frac{1}{\sigma}g'(\Phi_0)U_0 - \Delta r_0 \partial_{\varrho} \Phi_0 + \alpha \partial_t r_0 \partial_{\varrho} \Phi_0 &= 0. \end{aligned} \quad (22)$$

The indefinite integral of the heat equation here yields

$$K\partial_{\varrho} U_1 = -\frac{1}{2}v_0 \Phi_0 + c(t, s)$$

with  $v_0 = -\partial_t r_0$ . Combined with the matching conditions of order  $O(\varepsilon)$ ,

$$\lim_{\varrho \rightarrow \pm\infty} \partial_{\varrho} U_1 = \lim_{x \rightarrow \Gamma_{\pm}} \partial_n u_0$$

this yields

$$[K\partial_n u_0] = -lv_0,$$

this is the conservation of energy condition of leading order. The phase field equation here can be written as

$$L\Phi_1 = -\frac{1}{\sigma}g'(\Phi_0)U_0 - \Delta r_0 \partial_{\varrho} \Phi_0 + \alpha \partial_t r_0 \partial_{\varrho} \Phi_0 \quad (23)$$

with the differential operator  $L = \partial_{\varrho}^2 - f''(\Phi_0)$ . This equation has a solution, if the right hand side there is orthogonal in  $L_2(-\infty, +\infty)$  to the kernel of the differential operator  $L$ . Obviously,  $\partial_{\varrho} \Phi_0$  belongs to this kernel, hence the condition

$$\int_{-\infty}^{\infty} \partial_{\varrho} \Phi_0 \left( -\frac{1}{\sigma}g'(\Phi_0)U_0 - \Delta r_0 \partial_{\varrho} \Phi_0 + \alpha \partial_t r_0 \partial_{\varrho} \Phi_0 \right) d\varrho = 0$$

is valid. If the function  $g$  satisfies the scaling condition

$$\int_{-\infty}^{\infty} g'(\Phi_0) \partial_{\varrho} \Phi_0 d\varrho = g(1) - g(-1) = \int_{-\infty}^{\infty} (\partial_{\varrho} \Phi_0)^2 d\varrho, \quad (24)$$

then relation (24) takes the form

$$\frac{U_0}{\sigma} = -\Delta r_0 + \alpha \partial_t r_0 = -\kappa_0 - \alpha v_0. \quad (25)$$

This is the Gibbs-Thomson condition of leading order. A special choice of  $g$  that definitely satisfies condition (24) is given by

$$g'(\Phi_0) = \partial_{\varrho} \Phi_0. \quad (26)$$

If this is true, then the solvability condition (24) implies that the right hand side of (23) vanishes, and  $\Phi_1$  is a solution of

$$L\Phi_1 = 0.$$

This equation is supplemented by the condition  $\Phi_1(\varrho = 0) = 0$  — this is again a consequence of the choice of coordinate system — and the condition that  $\Phi_1$  remains bounded for  $\varrho \rightarrow \pm\infty$ . The resulting problem has only the trivial solution  $\Phi_1(\varrho) = 0$ . We continue with the inner expansion.

The phase field equation in the  $O(\varepsilon^2)$  **problem** is

$$\begin{aligned} -\partial_\varrho^2 \Phi_2 + \frac{1}{2} f'''(\Phi_0) \Phi_1^2 + f''(\Phi_0) \Phi_2 - \frac{1}{\sigma} g''(\Phi_0) U_0 \Phi_1 - \frac{1}{\sigma} g'(\Phi_0) U_1 \\ - \Delta r_1 \partial_\varrho \Phi_0 - \Delta r_0 \partial_\varrho \Phi_1 + \alpha \partial_t r_0 \partial_\varrho \Phi_1 + \alpha \partial_t r_1 \partial_\varrho \Phi_0 \\ + \alpha \partial_t \Phi_0 + \alpha \partial_t s_0 \partial_s \Phi_0 - |\nabla s_0|^2 \partial_s^2 \Phi_0 - \Delta s_0 \partial_s \Phi_0 = 0. \end{aligned} \quad (27)$$

Since  $\Phi_0$  depends on  $\varrho$  only, the last line here cancels. Under the condition (26) we have  $\Phi_1 = 0$  and the problem of order  $O(\varepsilon^2)$  is reduced to

$$\begin{aligned} L\Phi_2 &= -\frac{1}{\sigma} g'(\Phi_0) U_1 - \Delta r_1 \partial_\varrho \Phi_0 + \alpha \partial_t r_1 \partial_\varrho \Phi_0 \\ &= \left(-\frac{1}{\sigma} U_1 - \Delta r_1 + \alpha \partial_t r_1\right) \partial_\varrho \Phi_0. \end{aligned}$$

Once again, the right hand side of this equation must be orthogonal to  $\partial_\varrho \Phi_0$ ,

$$\int_{-\infty}^{\infty} \left(-\frac{1}{\sigma} U_1 - \Delta r_1 + \alpha \partial_t r_1\right) (\partial_\varrho \Phi_0)^2 d\varrho = 0, \quad (28)$$

or

$$\frac{\int_{-\infty}^{\infty} U_1 (\partial_\varrho \Phi_0)^2 d\varrho}{\int_{-\infty}^{\infty} (\partial_\varrho \Phi_0)^2 d\varrho} = -\sigma(\kappa_1 + \alpha v_1). \quad (29)$$

The left hand side here represents a weighted average of the corrector  $U_1$ , where the center of the interface is more heavily weighted. With the notation

$$\langle w \rangle := \frac{\int_{-\infty}^{\infty} w (\partial_\varrho \Phi_0)^2 d\varrho}{\int_{-\infty}^{\infty} (\partial_\varrho \Phi_0)^2 d\varrho},$$

we obtain by adding of (25) and (29)

$$\langle u_0 + \varepsilon u_1 \rangle = -\sigma((\kappa_0 + \varepsilon \kappa_1) + \alpha(v_0 + \varepsilon v_1)). \quad (30)$$

In this sense, the Gibbs-Thomson relation is valid up through the first two orders.  $\square$

**Remarks 1.** The  $O(1)$  level represents the sharp interface limit, where the interface width is actually equal to zero. Hence the Gibbs-Thomson relation holds in a pointwise sense. At the  $O(\varepsilon)$  level, the Gibbs-Thomson condition can be valid at most in a particular averaged sense. As it turns out here, the natural average is a weighted average with weight function  $(\partial_\varrho \Phi_0)^2$  so that the central region is heavily weighted.

2. Note that  $\Phi_1 = 0$  implies  $\varphi_1 = 0$  near the interface. Then (14) implies that  $u_1$  satisfies the heat equation on both sides of the interface, and we can assume

$$\partial_t u_1 = \nabla \cdot (K \nabla u_1).$$

If the initial and boundary conditions are independent of  $\varepsilon$ , then  $u_1$  satisfies the initial condition  $u_1(0, x) = 0$  and the boundary condition  $u_1(t, x) = 0$  or  $K \partial_n u_1(t, x) =$

0 for  $x \in \partial\Omega$ . In this case the available uniqueness results for parabolic equations show  $u_1 = 0$ . Hence the temperature field would be also accurate to second order.

As a conclusion to this asymptotics, we propose to use the relations (21) and (26),

$$\partial_\rho^2 \Phi_0 = f'(\Phi_0), \quad \partial_\rho \Phi_0 = g'(\Phi_0)$$

for the construction of efficient phase field models. These are two relations for the three functions  $\Phi_0$ ,  $f$  and  $g$ , and we may use them in order to define two of the functions in terms of the third one. For example, we may choose a certain shape transition function  $\Phi_0$  for the phase transition and then compute  $f$  and  $g$ . The functions  $f$  and  $g$  are then defined up to (unimportant) constants on the domain  $(-1, 1)$  at least (for a correct choice of  $\Phi_0$ , that means  $\Phi_0(+\infty) = 1$  and  $\Phi_0(-\infty) = -1$ ). They must be extended in a suitable way to the real line  $\mathbb{R}$ .

**3. Examples.** In the classical case, as mentioned above, the functions  $f$  and  $g$  are defined by

$$f(\varphi) = \frac{1}{2}(\varphi^2 - 1)^2, \quad g(\varphi) = \frac{2}{3}\varphi.$$

Here, equation (26) is not satisfied, hence the first order correction  $\Phi_1$  does not cancel. Moreover, the minima of the combined potential  $\varphi \mapsto f(\varphi) - \sigma^{-1}\varepsilon g(\varphi)u_0$  are not kept at  $\pm 1$ . This may lead to numerical inaccuracies, in particular for values of  $\varepsilon/\sigma$  that are not small.

Caginalp and Chen [4] proved the asymptotics for a spectrum of models so that  $f$  and  $g$  could be chosen from a set of functions for convenience in terms of either mathematical proofs or computations. In particular, one such choice, which we denote by CC1 is:

$$f(\varphi) = \frac{1}{2}(\varphi^2 - 1)^2 \quad \text{and} \quad g'(\varphi) = \frac{5}{4}(1 - \varphi^2)^2. \quad (31)$$

This type of choice fixes the roots for  $\varphi$  at exactly  $+1$  and  $-1$ , rather than allowing the phases to vary, as in the classical model. It has the computational convenience that one does not need to choose  $\varepsilon$  much smaller than the capillary length associated with the surface tension. This choice does not satisfy (26), so that the  $O(\varepsilon)$  term in the interface velocity is present. We use this as a prototype of a model with fixed roots and the presence of  $O(\varepsilon)$  terms.

If we choose the same function  $g$  as in CC1 and compute the double well potential  $f$  in such a way that condition (26) is satisfied, we obtain the model CC2 [5]:

$$f(\varphi) = \frac{1}{2}(\varphi^2 - 1)^4, \quad g'(\varphi) = (1 - \varphi^2)^2.$$

This models serves as a prototype satisfying the fixed root condition as well as (26).

Models with fixed roots have been used in other works. In particular, Kobayashi [9] proposed the functions.

$$f(\varphi) = \frac{1}{2}(\varphi^2 - 1)^2, \quad g(\varphi) = \frac{1}{3}\varphi(3 - \varphi^2).$$

It turns out that these functions also satisfy (26). Fabbri and Voller [8] compared numerical computations with the classical potential and the potential of Kobayashi, and concluded that the latter leads to somewhat more accurate results.

Another possibility to construct phase field models is to prescribe a desired shape  $\Phi_0$  of the phase transition and then compute the corresponding potentials. We define below models that satisfy (26), have the features of fixed roots for  $\varphi$ , and, additionally, have large derivatives near the roots of  $\varphi$ .

**A model with sine function shaped phase transition.** If  $\Phi_0$  is given by

$$\Phi_0(x) = \begin{cases} \sin x & \text{for } |x| \leq \pi/2, \\ 1 & \text{for } x > \pi/2, \\ -1 & \text{for } x < -\pi/2, \end{cases}$$

then the constitutive functions are

$$f(\varphi) = \frac{1}{2}(1 - \varphi^2) \quad \text{and} \quad g'(\varphi) = \sqrt{1 - \varphi^2} \quad \text{for } |\varphi| \leq 1.$$

These functions must be extended in an appropriate manner to  $\varphi \notin [-1, 1]$ . Since the derivative  $f'(\pm 1)$  does not vanish, the extended  $f$  will be non-smooth. The extension of  $g$  is done by its values at  $\varphi = -1$  for argument  $\varphi < -1$  and at  $\varphi = 1$  for  $\varphi > 1$ . In the numerical examples performed later the functions

$$f(\varphi) = \begin{cases} \frac{1}{2}(1 - \varphi^2), & |\varphi| \leq 1, \\ \frac{1}{2}(\varphi^2 - 1), & |\varphi| > 1 \end{cases} \quad \text{and} \quad g'(\varphi) = \begin{cases} \sqrt{1 - \varphi^2}, & |\varphi| \leq 1, \\ 0, & |\varphi| > 1 \end{cases}$$

are employed. Another possibility would be to consider  $f$  as a double obstacle potential by prohibiting values of  $\varphi$  outside the interval  $[-1, 1]$ .

**A model with polynomial phase transition.** Choosing as shape of the phase transition the function

$$\Phi_0(x) = \begin{cases} \frac{1}{2}x(3 - x^2) & \text{for } |x| \leq 1, \\ 1 & \text{for } x > 1, \\ -1 & \text{for } x < -1, \end{cases}$$

leads to the relations

$$f'(\frac{1}{2}(3x - x^3)) = -3x \quad \text{and} \\ g'(\frac{1}{2}(3x - x^3)) = \frac{3}{2}(1 - x^2).$$

Since the function  $y(x) = 3x - x^3$  cannot be easily inverted, we do not present any closed form of  $f$  and  $g$ . The graphs of these functions are shown in Figure 1 (with reasonable extensions outside  $[-1, 1]$ ).

**4. Numerical examples.** In order to evaluate the presented models, we consider the sharp interphase formulation of a simple, one-dimensional phase transition problem,

$$\begin{aligned} \partial_t u &= \nabla \cdot (K \nabla u) \quad \text{in } \Omega, \\ u(t, x_I(t)) &= -\sigma(\alpha v + \kappa), \\ [K \partial_x u(t, x_I(t))] &= -lv. \end{aligned}$$

Here,  $\Omega$  is a bounded interval and  $x_I(t)$  denotes the position of the interphase at time  $t$ . The initial and boundary data are chosen such that this problem has an

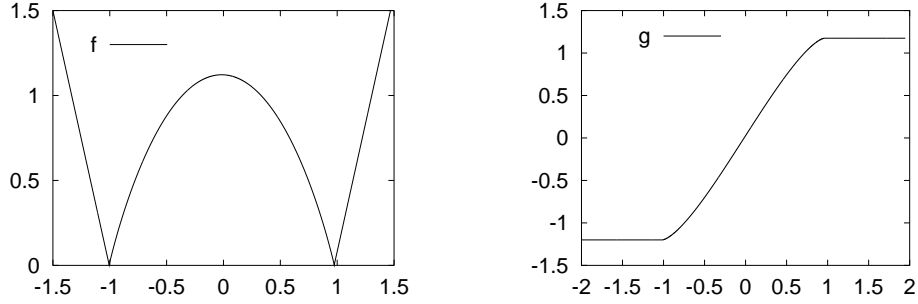


FIGURE 1. Potentials for polynomial transition shape

exact solution with constant interphase velocity  $v$  and constant temperature in the liquid domain. This leads to the temperature field,

$$u(t, x) = \begin{cases} -\sigma\alpha v + (1 - e^{-(x-x_I(t))v/K}), & x < x_I(t), \\ -\sigma\alpha v, & x \geq x_I(t), \end{cases} \quad (32)$$

with interphase position  $x_I(t) = x_0 + vt$ , from which the required initial data and boundary data follow. The data of the examples to be presented are  $\Omega = [0.0, 0.05]$ ,  $\sigma = 2.83 \cdot 10^{-7}$ ,  $\alpha = 10^6$ ,  $x_0 = 0.01$ ,  $K = 1.147 \cdot 10^{-3}$ ,  $l = 1$ ,  $v = 0.05$ .

No.	$\varepsilon$	$n$	$\Delta t$
1	$5 \cdot 10^{-3}$	500	$10^{-3} / 10^{-4}$
2	$2 \cdot 10^{-3}$	500	$10^{-3} / 10^{-4}$
3	$1 \cdot 10^{-3}$	500	$10^{-3} / 10^{-4}$
4	$5 \cdot 10^{-4}$	500	$10^{-3} / 10^{-4}$
5	$5 \cdot 10^{-4}$	1000	$10^{-3} / 10^{-4}$
6	$2 \cdot 10^{-4}$	2000	$1 \cdot 10^{-4}$
7	$2 \cdot 10^{-2}$	25	$1 \cdot 10^{-4}$
8	$1 \cdot 10^{-2}$	50	$1 \cdot 10^{-4}$
9	$5 \cdot 10^{-3}$	100	$1 \cdot 10^{-4}$
10	$2.5 \cdot 10^{-3}$	200	$1 \cdot 10^{-4}$
11	$1.25 \cdot 10^{-3}$	400	$1 \cdot 10^{-4}$
12	$6.25 \cdot 10^{-4}$	800	$1 \cdot 10^{-4}$
13	$3.725 \cdot 10^{-4}$	1600	$1 \cdot 10^{-4}$
14	$1.5625 \cdot 10^{-4}$	3200	$1 \cdot 10^{-4}$
15	$1 \cdot 10^{-4}$	4000	$1 \cdot 10^{-4}$
16	$1 \cdot 10^{-4}$	8000	$1 \cdot 10^{-5}$
17	$5 \cdot 10^{-4}$	8000	$5 \cdot 10^{-6}$
18	$8 \cdot 10^{-5}$	6000	$2.5 \cdot 10^{-5}$
19	$4 \cdot 10^{-5}$	12000	$2.5 \cdot 10^{-5}$

TABLE 1. Examples

The discretization of the phase field model is done by piecewise linear finite elements on a uniform discretization of the interval into  $n$  elements, and a semi-implicit time discretization with time step  $\Delta t$ . The phase field equation is solved with the temperature data from the previous time step. The nonlinear functions  $f'$

No.	Classic	Kobayashi	CC 1	CC 2	Sine Function	Polynomial
1	0.016707	0.029779	0.023897	0.024863	0.029816	0.029960
2	0.016794	0.029826	0.022885	0.024276	0.029927	0.029987
3	0.017655	0.029871	0.024380	0.025751	0.029955	0.029987
4	0.013668	0.029169	0.026151	0.027356	0.029985	0.029997
5	0.013727	0.029428	0.026185	0.027384	0.029985	0.030004
6	0.020721	0.029834	0.028429	0.029137	0.030002	0.030017
7	0.021434	0.031296	0.030824	0.031301	0.031299	0.031538
8	0.018183	0.030103	0.027973	0.028705	0.030122	0.030367
9	0.016700	0.029806	0.024132	0.025199	0.029830	0.029965
10	0.016616	0.029826	0.023110	0.024597	0.029947	0.030009
11	0.017320	0.029899	0.024303	0.025810	0.029938	0.029983
12	0.018432	0.029526	0.026047	0.027332	0.029979	0.030002
13	0.019785	0.029630	0.027257	0.028279	0.029991	0.030005
14	0.021247	0.029929	0.028750	0.029366	0.030005	0.030026
15	0.022196	0.030082	0.029181	0.029673	0.030019	0.030058
16	0.022195	0.029989	0.029178	0.029671	0.030002	0.030007
17	0.023615	0.030005	0.029525	0.029919	0.030007	0.030013
18			0.029579	0.029957		
19			0.029660	0.030004		

TABLE 2. Position of interface at time  $t = 0.4$ 

and  $g'$  are linearized around the solution of the previous time step in the case of a smooth potential  $f$  or taken with their values from the previous time step in the case of a non-smooth potential. The time discretization of the linear (or linearized) terms is done by the Crank-Nicolson scheme. The heat equation is solved after the phase field equation, using the just computed phase field for the computation of the latent heat. The discretization parameters for the examples are described in Table 1.

In order to compare the different models, we show the computed position of the interphase — defined as point of zero of the phase field — at time  $t = 0.4$  for the different models and several selected discretization parameters. The exact interphase position (for the sharp interphase model) is  $x_I(0.4) = 0.3$ .

The results are depicted in Table 2. With the classical potential, none of the chosen discretizations gives a reasonably accurate position of the interface, because the ratio  $\varepsilon/\sigma$  is too big for the chosen data. For these data it is important to keep the roots of the potential at  $\varphi = \pm 1$ , as accomplished by all the other potentials. The biggest time step  $\Delta t = 10^{-3}$  cannot be used for the non-smooth potentials, because the method does not converge in this case. This is a consequence of the explicit time discretization of the non-linear terms used for these models. Therefore the time step  $\Delta t = 10^{-4}$  was employed there.

The results clearly indicate that the models satisfying condition (26) (that are the Kobayashi model, the CC2 model, the sine function model and the polynomial model) lead to an accurate prediction of the interface position for a much bigger value of  $\varepsilon$ , with a much coarser discretization, than the models not satisfying (26), in particular than model CC1. The non-smooth models (the sine function model and the polynomial model) perform equally well. Concerning computing time, the

evaluation of the potentials for the polynomial model turned out to be quite expensive, the sine function model was considerably faster. An error of approximately one percent is obtained with the sine function model for discretization 8, by model CC1 for discretization 19 and by model CC2 for discretization 15. In other words, for this accuracy the sine function model needs only 1/200 of the elements compared to CC1 and 1/100 compared to CC2.

**5. Conclusions.** We have proposed a method for the choice of potentials in the phase field method which eliminates the leading order correction in the asymptotic expansion of the phase field. Numerical experiments in one space dimension indicate that models constructed from this method indeed show a better approximation to the sharp interface limit as measured by the interface position. These computations also indicate that non-smooth or double-obstacle potentials may be superior to smooth double well potentials in convergence speed although they introduce other difficulties due to the singular behavior.

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