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Triply periodic minimal surface using a modified Allen–Cahn equation

Yibao Li, Shimin Guo*

School of Mathematics and Statistics, Xi'an Jiaotong University, Xi'an 710049, China

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ABSTRACT

In this paper, we propose a fast and efficient model for triply periodic minimal surface. The proposed model is based on the Allen–Cahn equation with a Lagrange multiplier term. The Allen–Cahn equation has the motion of mean curvature. And the Lagrange multiplier term corresponding to the constant volume constraint also relates to the average of mean curvature. By combining two terms, the mean curvature will be constant everywhere on the surface at the equilibrium condition. The proposed numerical method with the second-order accuracy of time and space exhibits excellent stability. In addition, the resulting discrete system is solved by a fast numerical method such as a multigrid method. Various numerical experiments are performed to demonstrate the accuracy and robustness of the proposed method.

1. Introduction

Constant minimal surface raised widely as natural or man made structures are with nonzero constant mean curvature everywhere on the surface [1]. The special constant minimal surfaces with the mean curvature are zero, called minimal surfaces. If a minimal surface has space group symmetry, is periodic in three independent directions, and is often called triply periodic minimal surfaces [2,3]. Triply-periodic minimal surfaces [4–7] are of special interest to physical scientists, materials scientists, biologists, and mathematicians, because the geometry of triply periodic minimal surfaces strongly influences the physical properties of the material. Furthermore besides the beauty of periodic property, triply-periodic minimal surfaces are efficient partitioners of congruent spaces [8]. Therefore triply periodic minimal surface appears in a variety of physical structures such as bicontinuous mixtures, detergent films, lyotropic colloids, and biological systems. Many approaches are proposed to study discrete triply periodic constant minimal surfaces [9–23]. For example, Siem and Carter [13] investigated the stability of six triply periodic surfaces of constant mean curvature by using the Surface Evolver, which is a computer program that minimizes the energy of a surface subject to constraints [14]. Große-Brauckmann and Wohlgemuth [15] proved that the gyroid is the only known embedded triply periodic minimal surface with triple junctions and has constant mean curvature companions.

Yoo [16] described a triply periodic minimal surfaces with mesh surface using conventional marching cube algorithm, and proposed various related algorithms for generating complete solid model for various applications. Based on a hybrid method of triply periodic minimal surface and distance field, Yoo [17] also presented an effective method for the

* Corresponding author.
E-mail addresses: yibaoli@mail.xjtu.edu.cn (Y. Li), gsm861@126.com, shiminguo@mail.xjtu.edu.cn (S. Guo).
URL: http://gr.xjtu.edu.cn/web/yibaoli (Y. Li)

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three dimensional porous scaffold design of human tissue. Qi and Wang [18] proposed a periodic surface model, which generate approximately triply periodic minimal surfaces, to assist the construction of nano structures parametrically for computer-aided nano design. Based on a novel use of the centroidal Voronoi tessellation optimization framework, Pan et al. [1] present a new method for modeling discrete constant mean curvature surfaces. Over surface meshes, a sixth-order geometric evolution equation was performed to obtain the minimal surface [19]. Jung and Torquato [20] studied Stokes slow through triply porous media, whose interfaces are the triply periodic minimal surfaces, and explored whether the minimal surfaces are optimal for flow characteristics. Using a first-passage time method, Gevertz and Torquato computed the mean survival time of a Brownian particle for a wide class of triply periodic porous media, including minimal surfaces [21].

Using a variational level-set method formulation, Jung et al. [22] present a theoretical characterization of and a numerical algorithm for computing the triply periodic minimal surfaces. Yang et al. [23] generated triply periodic constant mean curvature surfaces using a Cahn–Hillard method like level set function. Starting from the periodic nodal surface approximation to minimal surfaces, they can generate various constant mean curvature surfaces with given volume fractions. Compared with the level set approach [22], their model is faster and more efficient. However, the computational cost for computing the Cahn–Hilliard equation, which has a fourth-order term, is certainly high compare to computing the second-order derivative term.

In this paper, we present a new phase-field approach for minimizing the triply periodic surfaces by using a modified Allen–Cahn equation. The proposed method has two terms. One is the Allen–Cahn equation [24], which has the motion of mean curvature [25–27]. The other term is the Lagrange multiplier term, which is corresponding to the constant volume constraint and relates to the average of mean curvature. By combining two terms, the mean curvature will be constant everywhere on the surface at the equilibrium condition. The proposed scheme, derived by combining the Adams–Bashforth method and linearly stabilized splitting scheme, is second-order accuracy of time and space. The resulting discrete system allows large time step and is solved by a multigrid method. We perform various numerical experiments such as: evolution of constant mean curvature surface, convergence test, stability test, generation of triply periodic constant mean curvature surfaces, comparison with previous model, and multiple triply periodic constant mean curvature surface simulations. All the simulations show that the proposed method is accuracy and robustness.

This paper is organized as follows. In Section 2, we review two models for minimizing the triply periodic minimal surfaces and describe our proposed method in detail. In Section 3, we describe the computationally efficient method. In Section 4, we perform some characteristic numerical experiments for minimal surface. Finally, conclusions are given in Section 5.

2. Description of the previous models

In this section, we briefly review two approaches such as level-set method [22], Cahn–Hillaird method [23], and describe our proposed method for triply periodic minimal surfaces in detail.

2.1. Variational level-set model

Jung et al. [22] study triply-periodic surfaces with minimal surface area under a constraint in the volume fraction of the regions (phases) that the surface separates. Using a variational level set method formulation, they present a theoretical characterization of and a numerical algorithm for computing these surfaces. They defined $\phi(\mathbf{x})$ on the domain Ω to represent the surface $\Gamma = \{\mathbf{x} : \psi(\mathbf{x}) = 0\}$, the inside of the surface $\{\mathbf{x}\colon \phi(\mathbf{x}) > 0\}$, and the outside $\{\mathbf{x}\colon \phi(\mathbf{x}) < 0\}$. Here ϕ is approaching to a signed distance function. The mean curvature κ is defined as

$$\kappa(\phi) = \nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right). \tag{1}$$

Their approach follows the work of Osher and Santosa [28], which evolves ϕ along steepest descent directions using the evolution equation:

$$\phi_t = v(\phi)|\nabla\phi|. \tag{2}$$

Here the velocity field $v(\mathbf{x}, t)$ is chosen as

$$v(\phi) = \kappa(\phi) - \lambda, \tag{3}$$

where λ is the average value of the mean curvature over the surface:

$$\lambda = \frac{\int_\Gamma \kappa \,\mathrm{d}s}{\int_\Gamma \mathrm{d}s} = \frac{\int_\Omega \kappa\,\delta(\phi)\,\mathrm{d}x}{\int_\Omega \delta(\phi)\,\mathrm{d}x}. \tag{4}$$

Here $\delta(\mathbf{x})$ is the Dirac delta function. Then Eqs. (2)–(4) imply that in the equilibrium condition, the mean curvature is constant over the entire surface, i.e., $\kappa(\phi) = \lambda$. Note that in [22], the authors proved that with the definition of λ in Eq. (4), the level set ϕ satisfies the volume fraction. The volume fraction $V(\phi)$ is defined as $V(\phi) = \int_\Omega (1 - H(\phi))dx$ and $H(\phi)$ is the Heaviside function. However, in numerical simulations, the iterates of the level set ϕ eventually fail to remain the volume fraction conservation [22]. Then they use a Newton iteration to enforce the volume fraction to be the volume fraction of the