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A high-order boundary integral method for surface diffusions on elastically stressed axisymmetric rods

Xiaofan Li [a,*], Qing Nie [b]

[a] Department of Applied Mathematics, Illinois Institute of Technology, 10 West 32nd Street, Chicago, IL 60616, USA
[b] Center for Mathematical and Computational Biology, Department of Mathematics, University of California, Irvine, CA 92697-3875, USA

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ABSTRACT

Many applications in materials involve surface diffusion of elastically stressed solids. Study of singularity formation and long-time behavior of such solid surfaces requires accurate simulations in both space and time. Here we present a high-order boundary integral method for an elastically stressed solid with axi-symmetry due to surface diffusions. In this method, the boundary integrals for isotropic elasticity in axi-symmetric geometry are approximated through modified alternating quadratures along with an extrapolation technique, leading to an arbitrarily high-order quadrature; in addition, a high-order (temporal) integration factor method, based on explicit representation of the mean curvature, is used to reduce the stability constraint on time-step. To apply this method to a periodic (in axial direction) and axi-symmetric elastically stressed cylinder, we also present a fast and accurate summation method for the periodic Green's functions of isotropic elasticity. Using the high-order boundary integral method, we demonstrate that in absence of elasticity the cylinder surface pinches in finite time at the axis of the symmetry and the universal cone angle of the pinching is found to be consistent with the previous studies based on a self-similar assumption. In the presence of elastic stress, we show that a finite time, geometrical singularity occurs well before the cylindrical solid collapses onto the axis of symmetry, and the angle of the corner singularity on the cylinder surface is also estimated.

1. Introduction

Since the work by Nichols and Mullins [19], the deformation of a heated solid due to surface diffusion has been under many studies because of its broad applications. Driven by surface energy only (without elasticity), a thin solid cylinder is unstable to axi-symmetric perturbations when the wavelength exceeds the circumference of the unperturbed cylinder, and will pinch off forming a chain of spheres. The axi-symmetric pinchoff is self-similar and the cylinder forms conical shape at the pinchoff whose cone angle is universal, independent of the initial shape (for a review and the references, see Bernoff et al. [2]).

In the presence of stress in the solid, Asaro and Tiller [1] studied the surface evolution of a semi-finite elastic space subjected to a non-hydrostatic stress in two dimensions. Grinfeld [8] investigated the instability of the interface between a non-hydrostatic stressed elastic body and a melt. Spencer et al. [30] discussed the stability of a vapor-film interface and the effect of misfit strain. Chiu and Gao [4] considered the evolution of cycloid-type surfaces of a stressed elastic half-space. Spencer and Meiron [31] numerically simulated the nonlinear evolution of the stress-driven surface instability of a solid in two

* Corresponding author. Tel.: +1 312 567 5340.
E-mail addresses: lix@iit.edu (X. Li), qnie@math.uci.edu (Q. Nie).

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dimensions. Panat et al. [22] studied the growth of surface perturbations induced by surface diffusion and bulk diffusion in a stressed solid.

For an axisymmetric solid, the linear stability analysis in Colin et al. [5] and Kirill et al. [14] and the numerical simulation of the fully nonlinear evolution of an axisymmetric cylinder in Li and Nie [17] demonstrated that the system develops short-wavelength instability when the applied stress is beyond a critical value. To study whether the instability leads to pinchoff or development of geometrical singularities in finite time, accurate calculations of the interface curvature, the elasticity energy and the temporal dynamics are needed.

The boundary integral method, which reduces the boundary value problems to a system of integral equations on the surface (or a curve), is particularly convenient and efficient for boundary value problems where Green's functions are known. In two dimensions, state-of-art spectrally accurate boundary integral methods have been developed for a wide variety of applications (for a review, see [11]). In axisymmetric domains, for systems with static boundaries, low-order methods have long been used for elasticity [13,18,6]; for moving interface problems, the integral calculation is usually of low order in Stokes flows (e.g., [23,32]) which have integral kernels similar to the isotropic elasticity; and, the integral calculations can be high-order (or adaptive) in potential flows because the singular kernels have relatively simple form [21,20]. The complex singularity forms of the axisymmetric Green's functions in the boundary integral equation of the elasticity or Stokes flows (for example, the two types of singularities, $1/r$ and $\ln r$, cannot be explicitly separated from the kernels) prevents direct applications of any existing high-order integral quadratures. For general smooth boundaries in three dimensions, a high-order boundary integral method for elliptic boundary value problems is presented in Ying et al. [34].

In this paper, to solve boundary integral equations for isotropic elasticity equations in axisymmetric settings, we apply a modified alternating point quadrature along with Richardson extrapolations to obtain a series of quadratures that can be of any odd orders. Furthermore, when the Green's functions are periodic in the axial direction, the evaluation of kernels usually dominates the overall simulation. To overcome this, we present a fast and accurate evaluation algorithm for the kernels using asymptotic expansions of the summations in terms of the number of summation periods and applying a recursive extrapolation technique.

In addition, the evolution equation involves a fourth-order derivative term due to the surface diffusion, yielding a severe numerical stability constraint on the size of time-steps when explicit temporal schemes are applied. On the other hand, any fully implicit schemes are computationally expensive as it is necessary to solve a large nonlinear system at each time step. In this paper, we present a high-order temporal scheme for interfaces in axisymmetric geometry based on the local decomposition technique and integration factor methods [10,25]. In this method, the fourth derivative term is integrated (in time) explicitly such that the constraint on the time-step is reduced significantly without increasing any computational cost.

With high-order accuracy in both space and time for the boundary integral method, we are able to study singularity formation for an elastically stressed periodic cylinder. Through direct numerical simulations, we find that in absence of elasticity the cylinder surface pinches at the axis of symmetry in a finite time, and the form of singularity is consistent with a previous study based on assumption of self-similarity of interface near pinchoff [2]. In presence of elasticity, our numerical simulations show that the cylinder surface develops a corner singularity in a finite time before it collapses onto the line of symmetry.

The paper is organized as follows: In Section 2, we present the governing equations of the system in which the stressed solid is periodic in axial direction and subject to uni-axial stress. In Section 3, we derive the boundary integral formulations of the system. In Section 4, we present detailed description of the numerical methods. In Section 5, we investigate the nonlinear evolution of the stressed cylinder and the singularity formation of the surface using the developed numerical methods.

2. Governing equations

Consider the deformation of an infinite, axisymmetric cylinder Ω induced by surface diffusion. The solid is periodic along the axis of symmetry, as illustrated in Fig. 1. The surface of the cylinder, denoted by its cross section in the (x, y)-plane $\mathbf{x}(\alpha, t)$, evolves to minimize the sum of the surface energy and elastic energy ([14] and references therein) through

$$\frac{\partial \mathbf{x}}{\partial t} \cdot \mathbf{n} \equiv v_n = \nabla_s^2 (\beta g^{el} - \kappa), \tag{1}$$

where $\mathbf{n}$ is the unit vector normal to the surface, g^{el} is the elastic energy density, the dimensionless parameter β measures the relative strength of the elastic energy over the surface energy, and $\kappa = \nabla_s \cdot \mathbf{n}$ is the sum of the principle curvatures. Both g^{el} and β will be defined below.

The stress in the solid due to an external force with magnitude F along the x-axis, the axis of axi-symmetry, satisfies $\int_{\Omega_c} \mathbf{t}\, dA = F\mathbf{e}_1$, where Ω_c is any cross section of the solid with a plane perpendicular to x-axis, $\mathbf{t}$ is the traction and $\mathbf{e}_1 = (1, 0, 0)$ is the unit vector along x-axis. The solid is at mechanical equilibrium in absence of body forces, $\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$, where $\boldsymbol{\sigma}$ denotes the stress tensor. The surface of the cylinder satisfies the traction-free condition, i.e. $\mathbf{t} = \mathbf{0}$ on $\partial\Omega$. The relation between the stress and strain tensors follows Hooke's law for isotropic elasticity, i.e. $\sigma_{ij} = 2\mu\epsilon_{ij} + \lambda\epsilon_{kk}\delta_{ij}$, where μ and λ are the Lamé constants. Einstein summation notation is assumed in this study. The periodic boundary conditions require $\mathbf{u}(\mathbf{x} + L_p\mathbf{e}_1) - \mathbf{u}(\mathbf{x}) = U\mathbf{e}_1$ and $\mathbf{t}(\mathbf{x} + L_p\mathbf{e}_1) + \mathbf{t}(\mathbf{x}) = \mathbf{0}$ for any $\mathbf{x}$ in the solid, where U is a constant determined through F and L_P is the length of one period. Given F or U, the displacement $\mathbf{u}$ on the interface $\partial\Omega$ is calculated by solving the elasticity equations. Then, the elastic energy density $g^{el} = \frac{1}{2}\boldsymbol{\sigma} \cdot \boldsymbol{\epsilon}$ can be computed using a local coordinate transformation [12,27].