Mathematical modeling and numerical treatment of adhesion, exfoliation and collision

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1 Scalar problem

In this talk, we would like to treat mathematical modeling and numerical treatment of adhesion, exfoliation and collision. Phenomena of adhesion and exfoliation come from droplet motion on a plane. We describe the surface of droplet by using a graph of scalar function. For this problem, key words are 'volume constraint', 'free boundary' and 'potential energy'. The constraint produces a non-local term in the partial differential equations. Hence, we need to introduce variational method to these problems. Lagrangian will be

$$L(u) = \int_\Omega \big(- \chi_{u>0} u_t^2 + |\nabla u|^2 + Q\chi_{u>0}\big)\, dx, \tag{1}$$

where $\chi_{u>0}$ is the characteristic function and Q is a force of adhesion. If the droplet keeps its volume, we can get the following equation:

$$\chi_{u>0} u_{tt} = \Delta u - Q\chi'_{u>0} + \Big(\int_\Omega [u_{tt} u + |\nabla u|^2]\, dx \Big) \chi_{u>0}. \tag{2}$$

2 Shell bouncing problem

The model equation is derived by calculating the energy stored in the shell. The considered types of energy are stretching energy, bending energy, energy related to the compression of the enclosed gas, potential energy and kinetic energy. We assume that the strip of initial radius r_0 is bent to radius r and stretched by the ratio $\tilde{\mu}$. We adopt the following form of elastic energy

$$E_e(\boldsymbol{p}) = \frac{1}{24} kh^3 \int_0^{2\pi} (\kappa - \kappa_0)^2 |\boldsymbol{p}_\theta|\, d\theta + \frac{1}{2} kh \int_0^{2\pi} \Big(\frac{|\boldsymbol{p}_\theta|}{|\boldsymbol{q}_\theta|} - 1 \Big)^2 |\boldsymbol{q}_\theta|\, d\theta.$$

Denoting the mass density of the shell in equilibrium by σ, the local mass density of the shell $\boldsymbol{p}$ becomes $\sigma |\boldsymbol{q}_\theta| / |\boldsymbol{p}_\theta|$ and thus the kinetic energy is given by

$$E_k(\boldsymbol{p}) = \frac{1}{2} h \int_0^{2\pi} \sigma |\boldsymbol{q}_\theta|\, |\boldsymbol{p}_t|^2 \chi_{p^2>0}\, d\theta.$$

Physically, this corresponds to the assumption of zero reflection and infinite friction between the shell and the obstacle.

When the shell is closed, it is necessary to take into account also the energy related to the compression of the gas present inside the shell. The energy stored due to compression of the enclosed volume V of gas can now be calculated as minus the work done by pressure forces:

$$E_g(\boldsymbol{p}) = -\int_{V_0}^{V} P\,dV = -\int_{V_0}^{V} \Big\{P_0 + c_g\big(\frac{1}{V} - \frac{1}{V_0}\big)\Big\}\,dV = -P_0(V-V_0) - c_g\Big(1 - \frac{V}{V_0} + \ln\frac{V}{V_0}\Big). \tag{3}$$

The constant c_g is the product of the total mass of the gas and the square of the sound of speed. The equilibrium volume V_0 is known and the volume of $\boldsymbol{p}(t)$ is given by

$$V = \frac{1}{2}\int_0^{2\pi} (\boldsymbol{p}\cdot A\boldsymbol{p}_\theta)\chi_{p^2>0}\,d\theta.$$

In real situations, the impact of a shell is influenced by the action of gravity. Therefore, we introduce also the gravity potential of the shell

$$E_p(\boldsymbol{p}) = gh\int_0^{2\pi} \sigma|\boldsymbol{q}_\theta|p^2\chi_{p^2>0}\,d\theta.$$

Employing the obtained elastic, kinetic and gas energies, the action integral is written as

$$I(\boldsymbol{p}) = \int_0^T \big(E_e(\boldsymbol{p}) + E_g(\boldsymbol{p}) + E_p(\boldsymbol{p}) - E_k(\boldsymbol{p})\big)\,dt. \tag{4}$$

Applying Hamilton's principle, the governing equation for the free part of the shell is obtained from

$$\frac{d}{d\epsilon}I(\boldsymbol{p}+\epsilon\boldsymbol{\phi})\big|_{\epsilon=0} = 0 \qquad \forall\boldsymbol{\phi}\in\big[C_0^\infty\big((0,T)\times(0,2\pi)\cap\{p^2>0\}\big)\big]^2, \tag{5}$$

where I is the action functional defined in (4).

In the sequel, we shall use the notation $\rho(\theta) = |\boldsymbol{p}_\theta(\theta)|/|\boldsymbol{q}_\theta(\theta)|$ for the local relative density with respect to the equilibrium state.

Taking into account the influence of the obstacle on the computed energy, one may expect that the following equation expresses, in a rough approximation, the deformation of the whole shell:

$$\begin{aligned}\sigma\chi_{p^2>0}\boldsymbol{p}_{tt} \;=\; & \big\{-\tfrac{1}{12}kh^2\rho(\kappa_{ss}+\tfrac{1}{2}\kappa^3)\chi_{p^2>0} + \tfrac{1}{24}kh^2\kappa_0^2\rho\kappa - k\rho(\rho-1)\kappa\chi_{p^2>0}\big\}\boldsymbol{\nu}\\ & +\frac{\rho}{h}\big(P_0 + c_g(\tfrac{1}{V}-\tfrac{1}{V_0})\big)\chi_{p^2>0}\boldsymbol{\nu} + k\rho\rho_s\chi_{p^2>0}\boldsymbol{\tau} + g\sigma\chi_{p^2>0}\boldsymbol{e}_2.\end{aligned} \tag{6}$$

In our talk, we will explain how to treat the above equation numerically and will show the numerical result.

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