数理解析研究所講究録
第 1628 巻 2009 年 42-47

Discrete Morse flow for nonlocal problems

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Abstract. *The analysis of evolutionary nonlocal problems represented by volume-constrained motion is discussed. The variational approach called the discrete Morse semi-flow proves to be a suitable tool.*

In this contribution, we consider the constrained film motion described by the following equations:

$$\rho u_{tt}(t,x) = \gamma\Delta u(t,x) + \lambda(t) \qquad \text{for } (t,x) \in (0,T) \times \Omega \cap \{u > 0\}, \tag{1}$$

$$\frac{\gamma}{2}|\nabla u|^2 - \frac{\rho}{2}u_t^2 = Q^2 \qquad \text{on } (0,T) \times \Omega \cap \partial\{u > 0\}, \tag{2}$$

$$u(0,x) = u_0(x), \quad u_t(0,x) = v_0(x) \quad \text{in } \Omega. \tag{3}$$

Here u is a scalar function $(0,T) \times \Omega \mapsto \boldsymbol{R}$ expressing the shape of film, Ω is a domain in $\boldsymbol{R}^m$ and ρ, γ and Q are given positive constants. The parameter Q describes the adhesive or surface tension properties of the materials. The value of u is set to zero outside of $\{u > 0\}$ which is the set $\{(t,x) \in [0,T] \times \bar{\Omega};\ u(t,x) > 0\}$. Finally, λ is a Lagrange multiplier originating in the requirement of volume preservation

$$\int_\Omega u(t,x)\,dx = V \qquad \forall t \in [0,T], \tag{4}$$

and is defined by

$$\lambda = \frac{1}{V}\int_\Omega \left[\rho u_{tt}u + \gamma|\nabla u|^2\right]\,dx. \tag{5}$$

Typical phenomena described by these equations without the volume constraint are vibration and peeling of a film. The volume-preserving equation can model motion of bubbles and droplets attached to surfaces (i.e., obstacles).

These equations are derived by the following consideration. First, we suppose that the potential energy for the shape of the film is described by the formula

$$\int_\Omega \left(\frac{\gamma}{2}|\nabla u|^2 + Q^2\chi_{u>0}\right)dx,$$

where $\chi_{u>0}$ is the characteristic function of the set $\{u > 0\}$. We define the action intergral of the film as

$$J(u) = \int_0^T \int_\Omega \left(\frac{\gamma}{2}|\nabla u|^2 + Q^2\chi_{u>0} - \frac{\rho}{2}u_t^2\chi_{u>0}\right)dxdt. \tag{6}$$

Then we can derive the film equation (1) by calculating the first variation using volume-preserving perturbations

$$\frac{dJ\left(\frac{u+\delta\zeta}{1+(\delta/V)\int\zeta}\right)}{d\delta}\Bigg|_{\delta=0}=0$$

for any $\zeta \in C_0^\infty((0,T)\times\Omega\cap\{u>0\})$.

We also derive the free boundary condition (2) by the following calculation. Let $\eta \in C_0^\infty((0,T)\times\Omega, \boldsymbol{R}\times\boldsymbol{R}^m)$, $z=(t,x)\in(0,T)\times\Omega$, define $\tau_\delta(z)=z+\delta\eta$ and choose K_δ in such a way that the perturbation $K_\delta u(\tau_\delta^{-1}(z))$ preserves volume. By carrying out the inner variation

$$\frac{dJ(K_\delta u(\tau_\delta^{-1}(z)))}{d\delta}\Bigg|_{\delta=0}=0,$$

we get the free boundary condition (2).

We study these equations by the discrete Morse flow approach introduced first in [1]. The discrete Morse flow is a method that solves time-dependent problems by discretizing time and defining a sequence of minimization problems approximating the original problem. The corresponding minimizers are then interpolated with respect to time and discretization parameter is sent to zero. The advantage of this method over other approaches lies mainly in its constructivity and in the absence of restrictive assumptions, such as convexity.

We shall explain the idea on the example of the wave equation ([5]). We consider the following problem:

$$\begin{aligned}
u_{tt}(t,x) &= \Delta u(t,x) \quad \text{in } Q_T=(0,T)\times\Omega, && (7)\\
u(t,x) &= 0 \qquad\qquad \text{on } (0,T)\times\partial\Omega, && (8)\\
u(0,x) &= u_0(x), \quad u_t(0,x)=v_0(x) \qquad \text{in } \Omega. && (9)
\end{aligned}$$

First, we fix a natural number $N>0$, determine the time step $h=T/N$ and put $u_1(x)=u_0(x)+hv_0(x)$. Function u_0 corresponds to the approximate solution at time level $t=0$, while function u_1 is the approximate solution at time level $t=h$. We define the approximate solution u_n on further time levels $t=nh$ for $n=2,3,\ldots,N$, to be a minimizer of the following functional in $H_0^1(\Omega)$:

$$J_n(u)=\int_\Omega \frac{|u-2u_{n-1}+u_{n-2}|^2}{2h^2}\,dx+\frac{1}{2}\int_\Omega |\nabla u|^2\,dx. \tag{10}$$

We observe that the second term of the functional is lower-semicontinuous with respect to sequentially weak convergence in $H^1(\Omega)$ and the first term is continuous in $L^2(\Omega)$. The existence of minimizers then follows immediately from the fact that the functionals are bounded from below. This is a crucial advantage over the continuous version of this functional, the Lagrangian of the type (6).

As the next step, we define the approximate solutions $\bar{u}^h$ and u^h through interpolation of the minimizers $\{u_n\}_{n=0}^N$ in time:

$$\bar{u}^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ u_n(x), & t \in ((n-1)h, nh],\ n = 1, \dots, N, \end{cases} \tag{11}$$

$$u^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ \frac{t-(n-1)h}{h} u_n(x) + \frac{nh-t}{h} u_{n-1}(x), & t \in ((n-1)h, nh], n = 1, \dots, N. \end{cases}$$

Since u_n is a minimizer of J_n, the first variation of J_n at u_n vanishes. Thus, for any $\varphi \in H_0^1(\Omega)$ we have

$$\int_h^T \int_\Omega \Big[\frac{u_t^h(t) - u_t^h(t-h)}{h}\varphi + \nabla\bar{u}^h \nabla\varphi\Big]\, dx\, dt = 0 \qquad \forall\varphi \in L^2(0,T; H_0^1(\Omega)). \tag{12}$$

Now, we take the time step to zero. To be able to do so, some estimate on the approximate solutions is needed. We obtain the following energy estimate:

$$\|u_t^h(t)\|_{L^2(\Omega)} + \|\nabla\bar{u}^h(t)\|_{L^2(\Omega)} \le C_E \qquad \text{for a.e. } t \in (0,T), \tag{13}$$

where constant C_E depends on H^1-norms of the initial data but is independent of h. Thanks to estimate (13), we can extract a subsequence converging weakly to a function $u \in H^1(Q_T)$ and pass to limit in (12) as $h \to 0+$ to conclude that

$$\int_0^T \int_\Omega (-u_t\varphi_t + \nabla u \nabla\varphi)\, dx\, dt - \int_\Omega v_0\varphi(0,x)\, dx = 0 \quad \forall\varphi \in C_0^\infty([0,T) \times \Omega). \tag{14}$$

Moreover, it can be shown that u satisfies boundary condition (8) and remaining initial condition (9) in the sense of traces. Therefore, we have proved by the discrete Morse flow method that there exists a weak solution $u \in H^1(Q_T)$ to problem (7) - (9).

The method of discrete Morse flow can be naturally applied to nonlocal problems and extends even to free-boundary problems. The advantage of our approach regarding globally constrained problems lies in the fact that a semi-discretization of time allows us to use results from elliptic theory. Moreover, the variational principle enables us to deal with the constraint by incorporating it in the set of admissible functions. In other words, we minimize a functional corresponding to (10) in the set

$$\mathcal{K} = \{u \in H_0^1(\Omega); \int_\Omega u\, dx = V\}, \tag{15}$$

instead of minimizing in $H_0^1(\Omega)$. In this way, we avoid the direct treatment of the nonlocal term.

One of the important points in the construction of approximate solution of the type (11) to free boundary constrained problems is to show the continuity of the corresponding minimizers and thus justify that the sets $\{u^h > 0\}$ are open.

The discrete Morse flow method has been applied to the analysis of volume-constrained evolutionary problems. A list of the main results follows.

Theorem (parabolic problem, see [2])

$$
\begin{aligned}
u_t(t,x) - \Delta u(t,x) &= f(t,x,u) + \lambda(t), \quad \lambda = \frac{1}{V}\int_\Omega (u_t u + |\nabla u|^2 - f(u)u)\,dx, \\
u(t,x) &= g(t,x) \qquad\qquad t \in (0,T),\ x \in \partial\Omega, \\
u(0,x) &= u_0(x) \qquad\qquad x \in \Omega.
\end{aligned} \tag{16}
$$

If $u_0 \in H^1(\Omega) \cap L^\infty(\Omega)$ then under certain conditions on f and g, there exists a function $u \in H^1(Q_T)$, satisfying the boundary and initial conditions of (16) and the volume constraint (4) such that

$$
\int_0^T \int_\Omega (u_t\phi + \nabla u \nabla\phi - f(u)\phi)\,dx\,dt = \int_0^T \int_\Omega \lambda\phi\,dx\,dt,
$$

for each $\phi \in L^2(0,T;H_0^1(\Omega))$. Furthermore, the solution is unique and Hölder continuous.

Theorem (hyperbolic problem, see [3])

$$
u_{tt}(t,x) = \Delta u(t,x) + \lambda(u), \quad \lambda = \frac{1}{V}\int_\Omega (u_{tt}u + |\nabla u|^2)\,dx, \tag{17}
$$

$$
u(t,x) = g(t,x) \qquad \text{on } (0,T)\times\partial\Omega, \tag{18}
$$

$$
u(0,x) = u_0(x), \quad u_t(0,x) = v_0(x) \qquad \text{in } \Omega. \tag{19}
$$

There exists a weak solution whose properties depend on the regularity of initial data. For example, if u_0, v_0 belong to $H^1(\Omega)$ and $g = 0$, then weak solution is a function $u \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H_0^1(\Omega))$ satisfying $u(0) = u_0$ and the following identity for all test functions $\phi \in C_0^\infty([0,T)\times\Omega)$ with $\Phi = \int_\Omega \phi\,dx$

$$
\begin{aligned}
&\int_0^T \int_\Omega (-u_t\phi_t + \nabla u \nabla\phi)\,dx\,dt - \int_\Omega v_0\phi(0)\,dx \\
&\quad = \frac{1}{V}\int_0^T \int_\Omega (-u_t(u\Phi)_t + |\nabla u|^2\Phi)\,dx\,dt - \frac{1}{V}\int_\Omega u_0 v_0 \Phi(0)\,dx.
\end{aligned}
$$

In the end, let us consider a slow motion of a droplet attached to a plane with nonuniform surface tension. This motion can be modeled by a parabolic free boundary equation with nonlocal term:

$$
u_t(t,x) = \Delta u(t,x) - \mu(x)\chi_\varepsilon'(u(t,x)) + \chi_{u>0}\lambda(t) \quad \text{in } Q_T. \tag{20}
$$

The unknown function u represents the shape of the drop and χ_ε is a nondecreasing smoothing of the characteristic function of the set $\{u > 0\}$. This term comes from the requirement of fixed contact angle at the free boundary of the drop. The coefficient μ represents the changing surface tensions and λ is a nonlocal term of the form

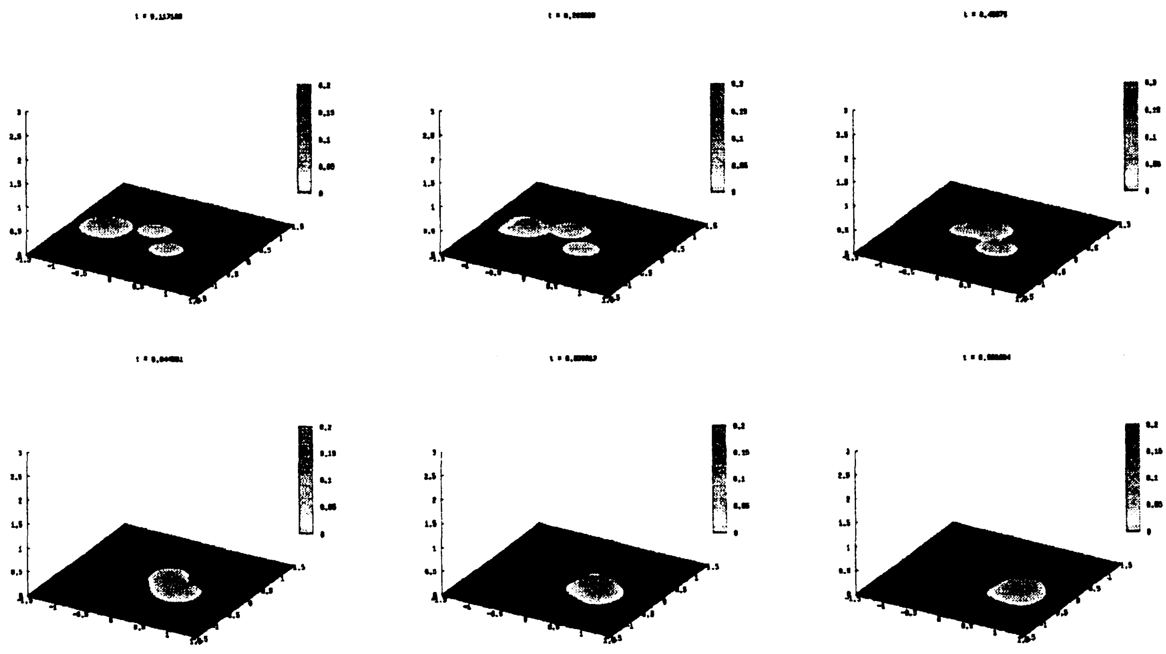
$$
\lambda = \frac{1}{V}\int_\Omega \left(u_t u + |\nabla u|^2 + \mu u \chi_\varepsilon'(u)\right) dx,
$$

originating in the volume constraint. For this type of problem we have the following result (see [4]).

Theorem (parabolic free boundary problem) *Let* $u_0 \in H_0^1(\Omega) \cap L^\infty(\Omega)$ *and* $\mu \in L^\infty(\Omega)$. *There exists a unique weak solution to the problem (20) that is Hölder continuous in* $[0,T] \times \bar{\Omega}$ *(if the initial datum is). The weak solution is defined only by test functions that have compact support inside* $\{u > 0\}$.

Apart from theoretical results, the proposed method is very efficient in the numerical solution of globally constrained evolutionary problems. In the numerical algorithm, time-discretized functional of the type (10) is discretized in space by FEM and minimized by the steepest descent method in the constrained set (15). The volume constraint represents a linear condition which leads to simple projections on a hyperplane.

We performed numerical computation for the problem (1)–(3) with added gravity term. This model expresses the motion of droplets on a slope. One can observe that the largest droplet starts moving since its gravity overpowers the surface tension forces. Then it catches up with the smaller droplets, fusing with them in turn.



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