Quantifying Tectonic and Geomorphic Interpretations of Thermochronometer Data: The Reconstruction of Mountain Surface

G. Bao[a], Y. Dou[e], T. Ehlers[b], P. Li[c], Y. Wang[d], Z. Xu[a]

[a]*Department of Mathematics, Michigan State University, East Lansing, MI 48824*
[b]*Department of Geology, University of Michigan*
[c]*Department of Mathematics, Purdue University*
[d]*Department of Mathematics, Fudan University, Shanghai, China*
[e]*Department of Mathematics, Harbin Institute of Technology, Harbin, China*

Abstract

Thermochronometer data offers a powerful tool for quantifying a wide range of geologic processes, such as the deformation and erosion of mountain ranges, paleotopography, hydrocarbon maturation, and forest fire frequency. With increasing interest to quantify a wider range of complicated geologic processes, more sophisticate techniques are in need. This paper is concerned with an inverse problem method for interpreting the thermonochronometer data quantitatively. Two novel models are proposed to simulate the thermal convection inside the mountain and the surface process, respectively. One is the heat transport process model which describes the change of temperature of rocks; while the other is surface process model which explains the change of surface of the mountain. New computational algorithms are developed for solving the inverse problem of the coupled system of these two models. The computational modeling should provide a systematic tool for restoring the historic geological process effectively.

Key words: Thermonochronometer, heat equations, inverse problem, variational method, iterative method, mountain surface.

Email address: zhengfu@math.msu.edu (Z. Xu)

1. Introduction

Recent years, there has been growing interest in developing suitable numerical methods for studying geology phenomena. A great deal of studies have been conducted, for example [13], [9]. Since the emerging of apatite (U-Th)/He thermochronometry as an important tool for quantifying the cooling history of rocks as they pass through the upper 1-3 km of the crust, the low closure temperature of this technique has attracted geomophologist and tectonocists with its application in interdisciplinary studies in the earth science, such as the landform evolution, structural geology, geomophology, geochemistry, petrology, and geodynamics [2], [17], [6]. Roughly speaking, thermochronometer data may be interpreted by measuring an age (or other related observables such as fission track lengths or noble gas release) from minerals extracted from rocks at or near the earth's surface. A thermonometer cooling age represents the time since a rock cooled below some effective closure temperature. These ages are influenced by either some events (e.g., fault motion, distribution of erosion in a catchment) or geologic processes (e.g., erosion, faulting, topographic change). In the latter case, which is closely related to our work in this paper, efforts are made to interpret the thermochronometer data to quantify the deformation, erosion, and topographic history of active mountain ranges. More specifically, we present in this paper a novel coupling of topographic evolution and 3D thermal and hydrologic models with inverse problem theory to restore the geologic processes in history. For thermal convection, the physical process is governed by

$$\rho c \left(\frac{\partial T}{\partial t} + \boldsymbol{v} \cdot \nabla T \right) = \nabla \cdot (k_1 \nabla T) + \rho H. \tag{1}$$

Explanation of the parameters will be given later in detail. This equation is a classic heat equation defined on the three dimensional region with moving boundary, considering heat transportation, diffusion and radiogenic effect. We also impose suitable boundary conditions based on the underlying physics. For surface process, we have another classic heat type equation, considering transportation by velocity field, diffusivity of nature, and fluvial process in place,

$$\frac{\partial S}{\partial t} = \nabla \cdot (k_2 \nabla S) + \boldsymbol{u} \cdot \nabla S + u_3 + a\sqrt{Q}\boldsymbol{d} \cdot \nabla S. \tag{2}$$

An interesting open problem is include the glacier melting process in the model, which would lead to highly nonlinear problem. Here $\boldsymbol{v} = (v_x, v_y, v_z)$

is the velocity, $\boldsymbol{u} = (v_x, v_y)$ and $u_3 = v_z$. For the inverse problem, the velocity $\boldsymbol{v}$ and surface $S(t, x, y)$ are the unknowns, which need to be reconstructed. The solution of the surface model serves as the moving boundary of the heat process. In our algorithm, we restore the velocity field by solving the inverse heat process model, and apply it as known to the surface model to obtain the initial surface by solving another inverse problem. This is carried out in an iterative fashion. To deal with the inverse problem entangled with a moving boundary, we freeze the boundary for a relatively short time period, by assuming that the mountain range does not change significantly in one thousand years.

A fundamental and yet often unquantified problem associated with themochronometer data is that interpretations of geologic processes influencing their thermal history are not unique. The non-uniqueness of interpretations stems from two typical sources: multiple thermal histories (e.g., slow protracted vs. rapid cooling) can produce the same thermochronometer age [16]; trade-offs between different physical preocesses (e.g., heat flow into the base of the crust and erosion rate) can produce similar thermal histories thereby adding uncertainty to interpretations [8]. Fortunately, in many cases, these uncertainties can be reduced by appropriate sampling and analysis of thermchronometer systems on the same sample. To quantify the geological process, we need to solve the equations (1) and (2) in a backward way. However the inverse problems of both the thermal convection and surface process are severely ill-posed, that is, small changes in the present temperature and surface may lead to large deviation of predicted velocity field and mountain surface in the past. The problem gets more serious in a large span of time simulation. There is sizable literature on the numerical solution of the backward heat equations (1) and (2), for example [4], [7]. Also, as well documented, the inverse problem to determine the coefficients of the lowest or leading terms for parabolic type equations is conditionally well-posed problem. Recent related results about the uniqueness and stability of recovery of certain coefficients of parabolic partial differential equations may be found in [3], [10], and [5]. We refer to [15] and [18] for numerical reconstructions where the Tikhonov regularization is used and [11] for the quasi-solution method.

Our goal of this work is to solve numerically the inverse problem of the coupled system with the finite element method, assuming that one measurement of the temperature is available at every point and the knowledge of the current surface profile. Our numerical results indicate that when the direction of the velocity field is known, (in practice, a priori guess of the direction of velocity field can be obtained by sampling) the reconstruction of the velocity field can be accurate. However, the reconstruction of the initial surface is accurate when the simulation time is short and less so for a long time simulation due to its ill-posedness. We also run the simulation for the coupled system, which incurs huge computational cost.

The rest of the paper is outlined as follows. We introduce the formulation of the problems in Section 2 and the algorithm for solving inverse problem in Section 3. In Section 4, our initial numerical results for the coefficient inverse heat transport problem and the inverse surface process problem are presented. We also demonstrate the numerical results for the coupled system.

2. Formulation

From the conservation of energy and Fourier's law for heat conduction that, at any point of the system $\mathbf{x} = (x, y, z) \in R^3$, the rate of change of temperature is proportional to the divergence of the heat flux:

$$\rho c \frac{dT}{dt} = \nabla \cdot (k \nabla T),$$

where ρ is the density of the material, in this case the rocks, c is the capacity of the system, k is the conductivity of the material and $T = T(t, \mathbf{x})$ is the temperature at $\mathbf{x} = (x, y, z)$ at time t.
If we consider the fact that rocks are transported at a velocity $\mathbf{v} = (v_x, v_y, v_z)$ and there exists a temperature gradient in the material along that direction, we have

$$\begin{aligned} \frac{dT}{dt} &= \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial t} + \frac{\partial T}{\partial z}\frac{\partial z}{\partial t} \\ &= \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} v_x + \frac{\partial T}{\partial y} v_y + \frac{\partial T}{\partial z} v_z \\ &= \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \end{aligned}$$

and

$$\rho c \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T\right) = \nabla \cdot (k \nabla T) \tag{3}$$

On the earth, most rocks contain a finite concentration of radioactive isotopes, such as U, Th, and K. The decay of these radioactive atoms gives rise to an increased kinetic energy. By adding the contribution of the source to (3), we have

$$\rho c(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T) = \nabla \cdot (k \nabla T) + \rho H,$$

where H is the rate of radiogenic heat production per unit mass. Let

$$D = \{(x, y)|0 \leq x \leq a, 0 \leq y \leq b\}, \quad \Omega = \{(x, y, z)|(x, y) \in D, 0 \leq z \leq S\},$$

where $S = S(t, x, y)$ is the surface of the mountain at time t. We consider the heat transport process model, which satisfies the following equation with proper boundary conditions

$$\begin{cases} \rho c \left(\dfrac{\partial T}{\partial t} + \boldsymbol{v} \cdot \nabla T \right) = \nabla \cdot (k_1 \nabla T) + \rho H, \\ T(t, x, y, S(t, x, y)) = T_a, \qquad (x, y) \in D, t_p \leq t \leq t_c, \\ T(t, x, y, 0) = T_m, \qquad (x, y) \in D, t_p \leq t \leq t_c, \\ \dfrac{\partial T}{\partial n}|_{(x,y) \in \partial D} = 0, \qquad (x, y) \in \partial D, t_p \leq t \leq t_c, \\ T(t_p, x, y, z) = T_p(x, y, z), \qquad (x, y, z) \in \Omega, t_p \leq t \leq t_c. \end{cases} \tag{4}$$

Here density of material ρ, capacity c, conductivity k_1, rate of radiogenic heat production per unit mass H could be obtained by experiments. The boundary value T_a is the temperature of air and T_m is the temperature at the bottom, usually the temperature of molten rock. These two parameters are known and initial temperature distribution $T_p(x, y, z)$ is also known. The vertical side boundaries are assumed to be conductively isolated, $\frac{\partial T}{\partial n} = 0$. For the inverse problem, the velocity $\boldsymbol{v}$ and surface $S(t, x, y)$ are unknown, which need be reconstructed. The measurement data is $T(t, \boldsymbol{x}_j(t)), j = 1, \cdots, m$, the history temperature data at points $\boldsymbol{x}_j(t)$. But actually even we know $\boldsymbol{x}_j(t_c))$, the current location of measurement points, we still do not know the history location of the measurement points $\boldsymbol{x}_j(t)), t_p \leq t < t_c$. To overcome this difficulty, it is assumed that the location is only changed by the velocity at this point

$$\boldsymbol{x}_j(t) = \boldsymbol{x}_j(t_c) - \int_t^{t_c} \boldsymbol{v} dt.$$

Another model is the Surface Process Model, where three mechanisms are involved: the hillslope process, the advection and uplift, and the fluvial process.

First, diffusion is used to represent a variety of surficial hillslope processes over long time scales, including regolith creep and mass wasting by bedrock-involved landslides, which describes the time dependent change on the surface of the earth,

$$\frac{\partial S}{\partial t} = \nabla \cdot (k \nabla S). \tag{5}$$

Here $S = S(t, \mathbf{x}), \mathbf{x} = (x_1, x_2) \in R^2$ is the height function of $\mathbf{x}$ at time t, and k is the diffusivity constant. If combined with an uplift by the velocity u_3 and a horizontal transport by the velocity $\mathbf{u} = (u_1, u_2)$, the equation (5) describing the change of surface can be changed to

$$\frac{\partial S}{\partial t} = \nabla \cdot (k \nabla S) + \mathbf{u} \cdot \nabla S + u_3.$$

Now we take the fluvial process into consideration. Define Q as the discharge L^3/t, ℓ as the direction of the river. Sediment is not considered in this model because bedrock channels have a sediment load less than the capacity and thus it is reasonable to believe there is no sediment storage. The bedrock incise at a rate of $\frac{\partial S}{\partial t}$, also taken to be proportional to stream power

$$\frac{\partial S}{\partial t} = \frac{k_f}{w} Q \frac{\partial S}{\partial \ell},$$

where w is the channel width and k_f is a proportionality constant. The channel width is assumed to be proportional to the square root of discharge

$$w = a\sqrt{Q}.$$

Finally

$$\frac{\partial S}{\partial t} = \nabla \cdot (k \nabla S) + \mathbf{u} \cdot \nabla S + u_3 + \frac{k_f}{a} \sqrt{Q} \frac{\partial S}{\partial \ell}.$$

By combining all of the factors considered above, we have the following equations for the surface process model

$$\begin{cases} \dfrac{\partial S}{\partial t} = \nabla \cdot (k_2 \nabla S) + \boldsymbol{u} \cdot \nabla S + u_3 + a\sqrt{Q}\boldsymbol{d} \cdot \nabla S, \\ \dfrac{\partial S}{\partial n}|_{\partial D} = 0, \\ S(t_p, x, y) = S_p(x, y), \qquad (x, y) \in D, t_p \leq t \leq t_c. \end{cases} \tag{6}$$

Here the diffusivity constant of hillslope k_2, proportional constant a, river channel discharge Q and direction $\boldsymbol{d}$ are known from historic data or by experiments. The functions $\boldsymbol{u}$ and u_3 are the velocity $\boldsymbol{v}$ on the surface. Our objective is to reconstruct $S_p(x,y)$ from $S_c(x,y)$.

The model problem is a coupled system because $\boldsymbol{u}$ and u_3 of the Surface Process Model come from the velocity $\boldsymbol{v}$ of the Heat Transport Process Model, while the top boundary of the domain for the Heat Transport Process Model comes from the solution of Surface Process Model. In the following, we abbreviate the Heat Transport Process Model and Surface Process Model by HTPM and SPM, respectively.

3. Algorithm

For simplicity, we assume that the velocity $\boldsymbol{v}$ is a piecewise constant function with respect to t

$$\boldsymbol{v}(t,x,y,z) = \boldsymbol{v}(t_i,x,y,z), t_i \le t < t_{i+1},$$

where $t_p = t_0 < t_1 < \cdots < t_N = t_c$ is a partition of $[t_p, t_c]$.
We also assume that

$$S(t,x,y,z) = S(t_i,x,y,z), t_i \le t < t_{i+1},$$

such that we can solve the forward problem of the heat transport process model in a fixed domain when $t_i \le t < t_{i+1}$.

The iteration is as follows:
First, we give the initial guess of the velocity $\boldsymbol{v}^{(k)}(t_i,x,y,z), i = 0,1,\cdots,N-1$ and the initial guess of the surface at time t_p: $S_p^{(k)}(x,y),(x,y) \in D$, where $S_p^{(k)}(x,y)$ is also the surface between time $[t_0,t_1]$, also denoted as $S_0^{(k)}(x,y),(x,y) \in D$. Here k is the count of the iterations, where $k=0$ at the beginning.
Next, we update $\boldsymbol{v}$ from $T(t,\boldsymbol{x}_j(t)), j = 1,\cdots,m$, assuming that $S_0(x,y)$ is fixed.
Then update $S(t_p,x,y)$ from the current surface $S(t_c,x,y)$, assuming that $\boldsymbol{v}$ is known.
Repeat the previous steps until certain stopping criterion is met.

Next the details for updating the velocity field and surface are discussed. To update S and V, we adopt the gradient method by minimizing the cost functional in the L_2 norm. To obtain the gradient of the cost functional, two backward heat type equations are solved.

3.1. Update $\mathbf{v}$ *when* $S_0(x, y)$ *is fixed*

Step 1: With the current $\boldsymbol{v}^{(k)}(t_i, x, y, z), i = 0, 1, \cdots, N-1$, we can obtain $\boldsymbol{u}(t_i, x, y)$ and $u_3(t_i, x, y)$ for $i = 0, 1, \cdots, N-1$. With the guess of initial surface $S_0^{(k)}(x, y)$, we solve the surface process model as a forward problem for

$$S_i(x, y) = S(t_i, x, y), (x, y) \in D, i = 0, 1, \cdots, N.$$

Step 2: Solve the heat transport process model for $t_0 \leq t \leq t_1$ with the velocity $\boldsymbol{v}^{(k)}(t_0, x, y, z)$. The initial temperature $T_0 = T_p$ is given. The temperature at t_1 is denoted as T_1 which is used as the initial value of the forward problem for $t_1 \leq t \leq t_2$.

Step 3: Update $\boldsymbol{v}^{(k)}(t_0, x, y, z)$ from the measurement data $T(t, \boldsymbol{x}_j(t)), t_0 \leq t \leq t_1$. The detailed algorithm for updating $\boldsymbol{v}^{(k)}(t_0, x, y, z)$ is provided below.

Step 4: Repeat Step 2 and Step 3 for $t_i \leq t \leq t_{i+1}, i = 1, 2, \cdots, N-1$.

Thus, we finish one cycle of iteration for updating $\boldsymbol{v}$.

To update $\boldsymbol{v}^{(k)}(t_i, x, y, z)$, we adopt a variational approach for the heat transport process model for $t_i \leq t \leq t_{i+1}$. Let $\tilde{\boldsymbol{v}} = \boldsymbol{v} + \delta \boldsymbol{v}$, T be the solution of the heat transport process model with the velocity $\boldsymbol{v}$ and $\tilde{T}$ be the solution with the velocity $\tilde{\boldsymbol{v}}$. Let $\delta T = \tilde{T} - T$. It is clear that the initial values are the same: $\tilde{T}_i = T_i$. Hence δT satisfies the following equations

$$\begin{cases} \rho c \left(\dfrac{\partial(\delta T)}{\partial t} + \boldsymbol{v} \cdot \nabla(\delta T) \right) = \nabla \cdot (k_1 \nabla(\delta T)) - \delta \boldsymbol{v} \cdot \nabla T, \\ \delta T(t, x, y, S(t, x, y)) = 0, \qquad (x, y) \in D, \\ \delta T(t, x, y, 0) = 0, \qquad (x, y) \in D, \\ \dfrac{\partial(\delta T)}{\partial n}|_{(x,y) \in \partial D} = 0, \qquad (x, y) \in \partial D, \\ \delta T(t_i, x, y, z) = 0, \qquad (x, y, z) \in \Omega, \end{cases} \tag{7}$$

where $\Omega = D \times S_i(x, y)$.

Define the cost functional

$$J(\boldsymbol{v}) = \frac{1}{2} \sum_{j=1}^{m} \int_{t_i}^{t_{i+1}} (T(t, \boldsymbol{x}_j) - Z(t, \boldsymbol{x}_j))^2 + \alpha_i \int_{\Omega} |\boldsymbol{v}|^2 = J_1 + J_2. \tag{8}$$

Since it is assumed that there is no movement in time $[t_i, t_{i+1}]$, $\boldsymbol{x}_j$ now is independent of time t for every j. To minimize the cost functional (8) by a gradient method, let

$$\zeta_j(t) = \zeta(t, \boldsymbol{x}_j) = T(t, \boldsymbol{x}_j) - Z(t, \boldsymbol{x}_j).$$

Thus

$$J_1(\tilde{\boldsymbol{v}}) - J_1(\boldsymbol{v}) = \frac{1}{2}\sum_{j=1}^{m}\int_{t_i}^{t_{i+1}} \delta T(t,\boldsymbol{x}_j)(\tilde{T}(t,\boldsymbol{x}_j) + T(t,\boldsymbol{x}_j) - 2Z(t,\boldsymbol{x}_j)).$$

Therefore

$$J_1^{'}(\boldsymbol{v})\delta\boldsymbol{v} = \int_{t_i}^{t_{i+1}}\sum_{j=1}^{m} T^{'}(t,\boldsymbol{x}_j)\delta\boldsymbol{v}\zeta_j(t) \tag{9}$$

or

$$J_1^{'}(\boldsymbol{v}) = \sum_{j=1}^{m} T^{'}(t,\boldsymbol{x}_j)\zeta_j(t),$$

where $T^{'}$ is the Frechet derivative with respect to $\boldsymbol{v}$. Consider the adjoint problem

$$\begin{cases} \rho c\left(\dfrac{\partial W}{\partial t} + \nabla\cdot(\boldsymbol{v}W)\right) = -\nabla\cdot(k_1\nabla W) - \displaystyle\sum_{j=1}^{m}\zeta_j(t)\delta(\boldsymbol{x}-\boldsymbol{x}_j), \\ W(t,x,y,S(t,x,y)) = 0, \qquad (x,y)\in D, \\ W(t,x,y,0) = 0, \qquad (x,y)\in D, \\ \boldsymbol{n}\cdot(\rho c\boldsymbol{v}W + k_1\nabla W)|_{(x,y)\in\partial D} = 0, \qquad (x,y)\in\partial D, \\ W(t_{i+1},x,y,z) = 0, \qquad (x,y,z)\in\Omega. \end{cases} \tag{10}$$

We have

$$\begin{aligned} \int_{t_i}^{t_{i+1}}\int_{\Omega} &\left\{W\left[\rho c\left(\frac{\partial(\delta T)}{\partial t} + \boldsymbol{v}\cdot\nabla(\delta T)\right) - \nabla\cdot(k_1\nabla(\delta T))\right]\right\} \\ + &\left\{\delta T\left[\rho c\left(\frac{\partial W}{\partial t} + \nabla\cdot(\boldsymbol{v}W)\right) + \nabla\cdot(k_1\nabla W)\right]\right\} \\ = &-\int_{t_i}^{t_{i+1}}\int_{\Omega}\left[W\delta\boldsymbol{v}\cdot\nabla T + \sum_{j=1}^{m}\delta T\zeta_j(t)\delta(\boldsymbol{x}-\boldsymbol{x}_j)\right]. \end{aligned}$$

Since

$$\int_{t_i}^{t_{i+1}}\int_{\Omega} W\rho c\frac{\partial(\delta T)}{\partial t} + \delta T\rho c\frac{\partial W}{\partial t} = \int_{\Omega}\rho c(W\delta T)|_{t_i}^{t_{i+1}} = 0,$$

$$\int_{t_i}^{t_{i+1}}\int_\Omega (W\rho c\boldsymbol{v}\cdot\nabla(\delta T)+\delta T\rho c\nabla\cdot(\boldsymbol{v}W)) = \int_{t_i}^{t_{i+1}}\rho c\int_{\partial\Omega}W\delta T\boldsymbol{v}\cdot\boldsymbol{n} = \int_{t_i}^{t_{i+1}}\delta T(\boldsymbol{n}\cdot\rho c\boldsymbol{v}W)|_{(x,y)\in\partial D}$$

and

$$\begin{aligned}&\int_{t_i}^{t_{i+1}}\int_\Omega(-W\nabla\cdot(k_1\nabla(\delta T))+\delta T\nabla\cdot(k_1\nabla W))\\ =& \int_{t_i}^{t_{i+1}}\int_{\partial\Omega}(-Wk_1\nabla(\delta T)\cdot\boldsymbol{n}+\delta Tk_1\nabla W\cdot\boldsymbol{n})\\ =& \int_{t_i}^{t_{i+1}}\delta T(\boldsymbol{n}\cdot k_1\nabla W)|_{(x,y)\in\partial D},\end{aligned}$$

it follows that

$$-\int_{t_i}^{t_{i+1}}\int_\Omega\delta\boldsymbol{v}\cdot\nabla TW = \int_{t_i}^{t_{i+1}}\int_\Omega\sum_{j=1}^m\delta T(t,\boldsymbol{x})\zeta_j(t)\delta(\boldsymbol{x}-\boldsymbol{x}_j), \quad (11)$$

$$= \int_{t_i}^{t_{i+1}}\sum_{j=1}^m\delta T(t,\boldsymbol{x}_j)\zeta_j(t). \quad (12)$$

By comparing (12) with (9), we have

$$J_1'(\boldsymbol{v}) = -\nabla TW.$$

Therefore, to obtain the gradient, we need to solve the adjoint problem (10), which is a backward heat equation.

3.2. Update $S_0(x,y)$ when **v** *is given*

We update $S_0(x,y)$ from the current surface $S_N(x,y) = S(t_c,x,y)$ while assuming that velocity $\boldsymbol{v}$ is given. Let $\tilde{S}_0(x,y) = S_0(x,y)+\delta S_0(x,y)$, where S is the solution of the surface process model with the initial value $S_0(x,y)$ and $\tilde{S}$ is the solution with the initial value $\tilde{S}_0$. Let $\delta S = \tilde{S}-S$. Then δS satisfies the following equations

$$\begin{cases}\dfrac{\partial(\delta S)}{\partial t} = \nabla\cdot(k_2\nabla(\delta S))+\boldsymbol{u}\cdot\nabla(\delta S)+a\sqrt{Q}\boldsymbol{d}\cdot\nabla(\delta S),\\ \dfrac{\partial(\delta S)}{\partial n}|_{\partial D}=0,\\ \delta S(t_0,x,y)=\delta S_0(x,y), \qquad (x,y)\in D, t_p\le t\le t_c.\end{cases} \quad (13)$$

Suppose that $S_c(x,y)$ is the measured surface at current time t_c and $S(t_N,x,y)$ is the numerically reconstructed surface with the initial value $S_0(x,y)$.

Define the cost functional

$$I(S_0) = \frac{1}{2}\int_D (S(t_N,x,y) - S_c(x,y))^2 + \beta \int_D |S_0|^2 = I_1 + I_2. \tag{14}$$

We apply the gradient method to minimize the cost functional defined in (14). Thus

$$I_1(\tilde{S}_0) - I_1(S_0) = \frac{1}{2}\int_D \delta S(t_N,x,y)(\tilde{S}(t_N,x,y) + S(t_N,x,y) - 2S_c(x,y)). \tag{15}$$

Therefore

$$I_1^{'}(S_0)\delta S_0 = \int_D S^{'}(t_N,x,y)\delta S_0(S(t_N,x,y) - S_c(x,y)),$$

where $S^{'}$ is the Frechet derivative with respect to the initial surface. To evaluate the gradient $I_1^{'}(S_0)$ of the functional $I(S_0)$, we introduce the adjoint problem

$$\begin{cases} \dfrac{\partial V}{\partial t} = -\nabla\cdot(k_2\nabla V) + \nabla\cdot(\boldsymbol{u}V) + \nabla\cdot(a\sqrt{Q}\boldsymbol{d}V), \\ \dfrac{\partial V}{\partial n}|_{\partial D} = 0, \\ V(t_c,x,y) = S(t_c,x,y) - S_c(x,y), \qquad (x,y)\in D. \end{cases} \tag{16}$$

Combining (13) with (16), we have

$$\begin{aligned} \int_{t_p}^{t_c}\int_D \quad & V\left[\frac{\partial(\delta S)}{\partial t} - \nabla\cdot(k_2\nabla(\delta S)) - \boldsymbol{u}\cdot\nabla(\delta S) - a\sqrt{Q}\boldsymbol{d}\cdot\nabla(\delta S)\right] \\ + \quad & \delta S\left[\frac{\partial V}{\partial t} + \nabla\cdot(k_2\nabla V) - \nabla\cdot(\boldsymbol{u}V) - \nabla\cdot(a\sqrt{Q}\boldsymbol{d}V)\right] = 0. \end{aligned}$$

Since

$$\int_{t_p}^{t_c}\int_D \delta S\frac{\partial V}{\partial t} + V\frac{\partial(\delta S)}{\partial t} = \int_D (V\delta S)|_{t_p}^{t_c} = \int_D ((S(t_c) - S_c)\delta S(t_c) - V(t_p)\delta S_0),$$

$$\int_{t_p}^{t_c}\int_D \delta S\nabla\cdot(k_2\nabla V) - V\nabla\cdot(k_2\nabla(\delta S)) = \int_{t_p}^{t_c}\int_{\partial D}\delta S k_2\frac{\partial V}{\partial n} - Vk_2\frac{\partial(\delta S)}{\partial n} = 0,$$

$$\int_{t_p}^{t_c}\int_D \delta S\nabla\cdot(\boldsymbol{u}V)+V\boldsymbol{u}\cdot\nabla(\delta S)=\int_{t_p}^{t_c}\int_{\partial D}\delta SV\boldsymbol{u}\cdot\boldsymbol{n}=0$$

and

$$\int_{t_p}^{t_c}\int_D \delta S\nabla\cdot(a\sqrt{Q}\boldsymbol{d}V)+Va\sqrt{Q}\boldsymbol{d}\cdot\nabla(\delta S)=\int_{t_p}^{t_c}\int_{\partial D}\delta Sa\sqrt{Q}\boldsymbol{d}\cdot\boldsymbol{n}=0,$$

we obtain

$$\int_D (S(t_c)-S_c)\delta S(t_c)=\int_D V(t_p)\delta S_0. \tag{17}$$

By comparing (17) with (15), we derivethe gradient of the cost functional as $I_1'(S_0)=V(t_p,x,y)$. Therefore, the gradient of the cost functional (14) can be evaluated through solving the adjoint problem (16).

3.3. A modification of the inverse problem for HTPM

It is evident that additional information on the data to be recovered certainly enhances the accuracy of the numerical reconstruction. For example, a priori knowledge (through sampling) of the direction or distribution of the velocity field can lead to the simplification

$$\boldsymbol{v}=v\cdot\boldsymbol{d},$$

where v is unknown but $\boldsymbol{d}$ is known. The governing equation (4) is replaced by a slightly modified version

$$\begin{cases}\rho c\left(\dfrac{\partial T}{\partial t}+v\boldsymbol{d}\cdot\nabla T\right)=\nabla\cdot(k\nabla T)+\rho H, & (x,y,z)\in\Omega,\ 0\le t\le t^*,\\ T(t,x,y,S(t,x,y))=T_a, & (x,y)\in D, 0\le t\le t^*,\\ T(t,x,y,0)=T_c, & (x,y)\in D, 0\le t\le t^*,\\ \dfrac{\partial T}{\partial n}|_{(x,y)\in\partial D}=0, & (x,y)\in\partial D, 0\le t\le t^*,\\ T(0,x,y,z)=T_0(x,y,z), & (x,y,z)\in\Omega, 0\le t\le t^*.\end{cases} \tag{18}$$

For the inverse problem, the observation data is one measurement of the temperature T at time t^*, which is denoted as $Z(x,y,z)$. Similarly, we define the cost functional

$$J(\boldsymbol{v})=\frac{1}{2}\int_\Omega (T(t^*;\boldsymbol{x})-Z)^2+\alpha\int_\Omega|\boldsymbol{v}|^2=J_1+J_2.$$

Let

$$\zeta = T(t^*; \boldsymbol{x}) - Z,$$

then

$$J_1(\tilde{\boldsymbol{v}}) - J_1(\boldsymbol{v}) = \frac{1}{2}\int_\Omega \delta T(t^*)(\tilde{T}(t^*) + T(t^*) - 2Z).$$

Hence

$$J_1^{'}(\boldsymbol{v})\delta\boldsymbol{v} = \int_\Omega T^{'}(t^*)\delta\boldsymbol{v}\zeta$$

or

$$J_1^{'}(\boldsymbol{v}) = T^{'}(t^*)\zeta.$$

Consider the adjoint problem

$$\begin{cases} \rho c\left(\dfrac{\partial W}{\partial t} + \nabla\cdot(\boldsymbol{v}W)\right) = -\nabla\cdot(k\nabla W), \\ W(t,x,y,S(t,x,y)) = 0, \qquad (x,y)\in D, \\ W(t,x,y,0) = 0, \qquad (x,y)\in D, \\ \boldsymbol{n}\cdot(\rho c\boldsymbol{v}W + k\nabla W)|_{(x,y)\in\partial D} = 0, \qquad (x,y)\in\partial D, \\ W(t^*,x,y,z) = \zeta, \qquad (x,y,z)\in\Omega. \end{cases} \tag{19}$$

We have

$$\begin{aligned} \int_0^{t^*}\int_\Omega \quad & \left\{W\left[\rho c\left(\frac{\partial(\delta T)}{\partial t} + \boldsymbol{v}\cdot\nabla(\delta T)\right) - \nabla\cdot(k\nabla(\delta T))\right]\right\} \\ + \quad & \left\{\delta T\left[\rho c\left(\frac{\partial W}{\partial t} + \nabla\cdot(\boldsymbol{v}W)\right) + \nabla\cdot(k\nabla W)\right]\right\} \\ = \quad & -\int_0^{t^*}\int_\Omega (W\delta\boldsymbol{v}\cdot\nabla T). \end{aligned}$$

Since

$$\int_0^{t^*}\int_\Omega\left(W\rho c\frac{\partial(\delta T)}{\partial t} + \delta T\rho c\frac{\partial W}{\partial t}\right) = \int_\Omega \rho c(W\delta T)|_0^{t^*} = \int_\Omega \rho c\zeta\delta T(t^*),$$

$$\begin{aligned} \int_0^{t^*}\int_\Omega (W\rho c\boldsymbol{v}\cdot\nabla(\delta T) + \delta T\rho c\nabla\cdot(\boldsymbol{v}W) \quad &= \quad \int_0^{t^*}\rho c\int_{\partial\Omega} W\delta T\boldsymbol{v}\cdot\boldsymbol{n} \\ &= \quad \int_0^{t^*}\delta T(\boldsymbol{n}\cdot\rho c\boldsymbol{v}W)|_{(x,y)\in\partial D} \end{aligned}$$

and

$$\begin{aligned}\int_0^{t^*}\int_\Omega & - \quad W\nabla\cdot(k\nabla(\delta T)) + \delta T\nabla\cdot(k\nabla W)\\ &= \int_0^{t^*}\int_{\partial\Omega}(-Wk\nabla(\delta T)\cdot\boldsymbol{n} + \delta Tk\nabla W\cdot\boldsymbol{n})\\ &= \int_0^{t^*}\delta T(\boldsymbol{n}\cdot k\nabla W)|_{(x,y)\in\partial D},\end{aligned}$$

we obtain

$$-\int_0^{t^*}\int_\Omega \delta\boldsymbol{v}\cdot\nabla TW = \int_\Omega \rho c\delta T(t^*)\zeta.$$

Thus

$$J_1'(\boldsymbol{v})\delta\boldsymbol{v} = -\frac{1}{\rho c}\int_0^{t^*}\int_\Omega \delta\boldsymbol{v}\cdot\nabla TW$$

or

$$J_1'(v) = -\frac{1}{\rho c}\boldsymbol{d}\cdot\nabla TW.$$

4. Numerical Results

In this section we present several numerical test results to validate our model. The following experimental data for parameters are used in the governing equation for our numerical computation purpose:

- Heat transport diffusivity: 32 km^2/myr.
- velocity: on the scale of 1.0 km/myr.
- ρ: 2700 kg/m^3.
- c: heat capacity 800 J/(kg K).
- H: radiogenic production 0.5 microwatt/m^3.
- $T_a = 293K$, $T_m = 1073K$.

For the numerical computation, we use the following setup:

- The computational domain: $x \in [0, 100]$ km, $y \in [0, 50]$ km, $z \in [0, S(x, y)]$ km; each time interval is separated into 20 time steps.

- The regularization parameter: $\alpha = 10^{-3}$, $\beta = 10^{-6}$.
- Measurement data: $T(t_c, \mathbf{x}_j(t_c))$, temperature on nodes in subsection 4.1.
- Measurement data: $S(t_c, x_j, y_j)$, lift of surface on nodes in subsection 4.2.
- Measurement data: $\{T(n\triangle t, \mathbf{x}_j(n\triangle t))\}|_{n=1}^{N}$ and $S(t_c, x_j, y_j)$ on nodes in subsection 4.3.

To create the mesh for the finite element method, we employ a simple and effective mesh generator in MATLAB by Persson and Strang [14] for 3D HTPM. In the spatial domain Ω, we choose the continuous piecewise linear polynomial. In the temporal domain, we use the backward Euler method. All of the numerical experiments are performed in a Window XP machine with an Inter(R) Pentium(R) 4 , 3.20GHz, 3.19 GHz CPU and 2.00GB of RAM.

4.1. Backward for HTPM

We run the numerical simulation on one time interval $t_c - \triangle t \leq t \leq t_c$, $t_c = 5 \times 10^5$, $\triangle t = 1 \times 10^5$.

Test 1 We begin with the simplest case in which the velocity field is composed of a two-component piecewise constant. The direction is also assumed to be known. The data to be restored is the magnitude. We use the heat transport model within the fixed domain to solve a coefficient inverse problem for reconstructing the simple velocity field. For simplicity, we assume zero velocity in the x direction, though our algorithm and computation may be extended to the three dimensional case. We use one measurement of the temperature at the end of time period for the observation. Figure 1 is the profile of the velocity field. Table 1 shows the reconstruction accuracy.

relative error	iterations	elements
$77\% \to 0.3\%$	27	17070

Table 1: Two component piecewise constant velocity field

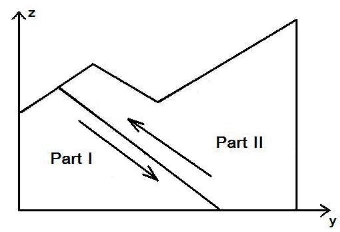

Figure 1: Two component piecewise constant velocity field

Test 2 The velocity field is assumed to be composed of four piecewise constants. Once again, the direction is known and the magnitude is what we need to reconstruct. Figure 2 and Table 2 show the velocity profile and accuracy of restoration, respectively.

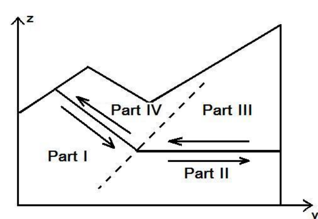

Figure 2: Four component piecewise constant velocity field

relative error	iterations	elements
84% $\rightarrow$ 0.5%	42	17070

Table 2: Four component piecewise constant velocity field

Test 3 As expected, the numerically recovered velocity field is consistent with the exact data for the last two setup. For now, we test our numerical method for a velocity field which is composed of four parts. For each part, the direction is unknown either. The result in Table 3 shows that the reconstruction is less accurate due to the more information to be restored. And it gets better when we drop the unresolved boundary layer or when we refine the mesh, which means more information at our disposal and high numerical accuracy.

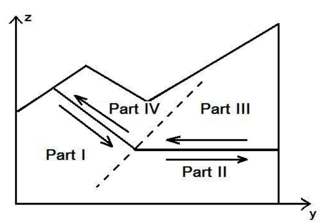

Figure 3: Four component piecewise constant velocity field

relative error	drop boundary	drop two layers	iterations	elements
87% → 37%	87% → 16%	87% → 8%	583	17070
87% → 24%	87% → 7%	87% → 3%	807	31687

Table 3: Four component piecewise variable velocity field

4.2. Model IV (Backward for SPM)

We run the numerical simulation on one time interval $t_c - \triangle t \leq t \leq t_c$, $t_c = 5 \times 10^5$, $\triangle t = 1 \times 10^5$. The algorithm for the surface process model is much simpler than for the heat transportation process model because the surface process model is a linear problem. Nevertheless, it is also a typical backward parabolic problem. The reconstruction of the initial value is extremely ill-posed. Although to reconstruct the initial value is not stable, the reconstruction at any time t, $t_p < t < t_c$, is better. The reconstruction is better if time t is closer to t_c. In this subsection, we present a numerical result at initial time and at half time. The initial surface is

$$S_p(x, y) = (\cos(\pi \times x/100) + \cos(\pi \times y/50)) \times 2 + 20.$$

Figure 4 shows the exact and reconstructed initial surface. Figure 5 shows the exact and numerically restored surface at the middle of this time period.

Table 4 shows the accuracy of restoring surface to the past.

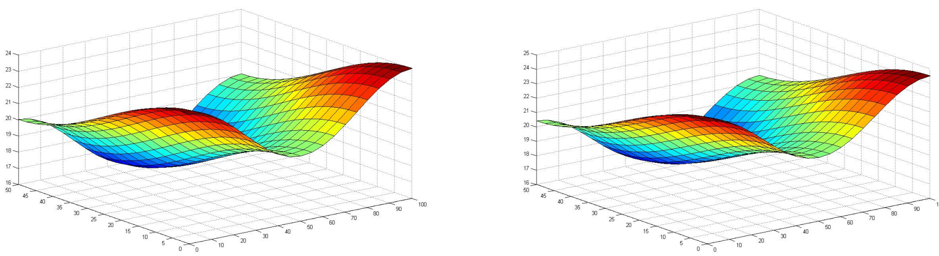

Figure 4: Left: Exact initial surface; Right: Reconstructed initial surface

initial guess	relative error	computational cost
$S(x, y) = 15$	$23\% \to 0.3\%$	13 seconds

Table 4: Accuracy of the reconstruction

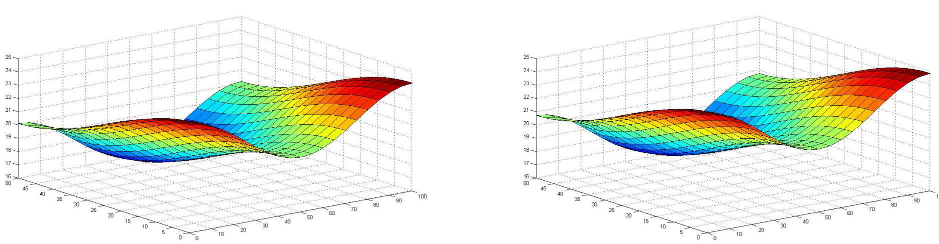

Figure 5: Left: Exact half-time surface; Right: Reconstructed half-time surface

4.3. Model V: The coupled system

We run the numerical simulation on one time interval $t_p = 0 \leq t \leq t_c$, $t_c = 5 \times 10^5$, $\triangle t = 1 \times 10^5$. For the coupled system, the main challenge is the slow convergence of the iterations, thus large computational cost. We test our method on the case that velocity field is composed of four parts, for each part the direction of the velocity is known. In order to test stability of the algorithm, we also add 5% random noise to the measurement data. We compare the two figures in Figure 7, the exact initial surface and the numerically reconstructed surface. It shows that the main feature of the surface is restored correctly and the accuracy shown in the Table 6 is satisfactory. Figure 6 is the velocity profile.

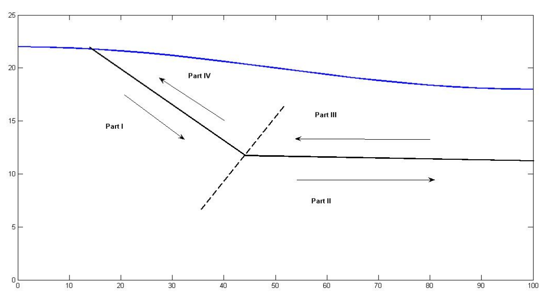

Figure 6: Four component piecewise constant velocity field

Time interval	v_y				v_z			
N	I	II	III	IV	I	II	III	IV
1	1	1.5	-2	-1.3	-1	0	0	1.3
2	0.8	1.5	-2	-1.4	-0.8	0	0	1.4
3	0.8	1.2	-1.7	-1.3	-0.8	0	0	-.3
4	1	1.5	-1.8	-1.5	-1	0	0	1.5
5	1.2	1.5	-2	-1.5	-1.2	0	0	1.5

Table 5: velocity field

We choose the velocity in the Table 5 as the exact velocity field, in which each row is corresponding to the velocity for one time interval.

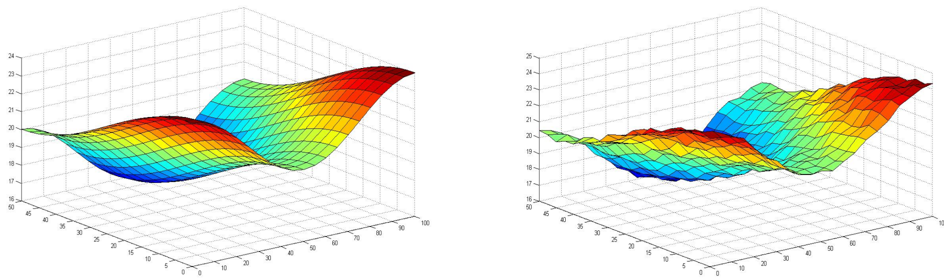

Figure 7: Left: Exact initial surface; Right: Reconstructed initial surface

initial guess	relative error	computational cost	elements
$S(x, y) = 15$	$23\% \rightarrow 2\%$	18 hours	17070

Table 6: Reconstruction without random noise to the the measurement data

5. Conclusion

Successful reconstruction of the mountain surface often provides geologists with a valuable perspective about the limit of the range that thermochronometer data can be interpreted. In this paper, we have presented a novel inverse problem method along with the new algorithms and numerical examples. Our method provides a solid and essential mean in understanding how to reconstruct the mountain surface of the past efficiently and accurately. We have also presented the mathematical model formulation by taking account of the main factors affecting temperature distribution in the mountain, such as heat transferring in the mountain, heat produced by the radiological element in rocks whose history temperature can be used for observation. As the initial step, we have tested our models on very simple cases to obtain promising numerical results. Even with a limited amount of data, our results have demonstrated the restored surface carries important features of the (exact) initial surfaces for the test problems. Our general computational approach may be extended to a range of other geodynamics.

Our long term objective is to develop a systematic tool for the understanding of dynamic geological processes influenced by thermal factors. A significant inherent challenge is to produce accurate numerical approximation of the large scale problem in the millions of years time span.

We conclude the paper by some general remarks about future directions along this line of research. There are many other factors affecting the temperature distribution that are neglected in our governing equations. An interesting future direction is to include also the melting effect which would lead to a highly nonlinear equation. The corresponding inverse problem for the nonlinear forward problem is at present completely open. Another interesting open problem is to numerically solve the problem with more realistic setups so that the measurement data is $T(t, \boldsymbol{x}_j(t)), j = 1, \cdots, m$, the history temperature data at rocks $\boldsymbol{x}_j(t)$ carrying radiogenic elements. Mathematically, an interesting problem is to study the uniqueness question for the coefficient inverse problem given the direction of the velocity field. There are also many challenging issues for developing fast and efficient algorithms for solving the large scale model problem.

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