FEM with Adjoint Method for Inverse Heat Conduction Problem

1 An Iterative Finite-Element Algorithm for Solving Two-Dimensional Nonlinear Inverse Heat Conduction Problems

1.1 Primal Problem

We have the primal problem which is the following system

$$\begin{cases}
\rho c(T) \frac{\partial T}{\partial t} = \nabla \cdot (\lambda(T) \nabla T) & (\mathbf{x}, t) \in (\Omega, \mathcal{T}) \quad \text{(a)} \\
T(\mathbf{x}, 0) = \tilde{Y}^{\xi} & \mathbf{x} \in \Omega \quad \text{(b)} \\
\lambda(T) \nabla T \cdot \mathbf{n} = q_u(\mathbf{x}, t) & (\mathbf{x}, t) \in (\Gamma_u, \mathcal{T}) \quad \text{(c)} \\
\lambda(T) \nabla T \cdot \mathbf{n} = q_g(\mathbf{x}, t) & (\mathbf{x}, t) \in (\Gamma_g, \mathcal{T}) \quad \text{(d)}
\end{cases}$$
(1)

In Eq.42, q_u is the unknown Neumann boundary condition on Γ_u while q_g is known on Γ_g .

1.2 Objective Function

From the primal problem, we define the objective function

$$\mathcal{J}(q_u) = \frac{1}{2} \int_0^{t_f} \int_{\Gamma_q} \left(T - Y^{\xi} \right)^2 d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} \left(q_u \right)^2 d\Gamma dt. \tag{2}$$

1.3 Sensitivity Problem

Next, we are going to derive the sensitivity problem. Firstly, we have the following definition

$$\theta(\boldsymbol{x}, t; q_u, \Delta q_u) = \lim_{\epsilon \to 0} \frac{T(\boldsymbol{x}, t; q_u + \epsilon \Delta q_u) - T(\boldsymbol{x}, t; q_u)}{\epsilon}, \tag{3}$$

it is clear that

$$T(\boldsymbol{x}, t; q_u + \epsilon \Delta q_u) \approx T(\boldsymbol{x}, t; q_u) + \epsilon \theta(\boldsymbol{x}, t; q_u, \Delta q_u).$$
 (4)

For simplicity,

$$T^+ := T(q_u + \epsilon \Delta q_u),$$

 $T := T(q_u).$

From Eq.42(a), we have

$$\rho c(T^+) \frac{\partial T^+}{\partial t} - \rho c(T) \frac{\partial T}{\partial t} = \nabla \left(\lambda(T^+) \nabla T^+ \right) - \nabla \left(\lambda(T) \nabla T \right).$$

Then

$$\rho c(T^{+}) \frac{\partial T}{\partial t} - \rho c(T) \frac{\partial T}{\partial t} + \epsilon \rho c(T^{+}) \frac{\partial \theta}{\partial t} = \nabla \left[\left(\lambda(T^{+}) - \lambda(T) \right) \nabla T + \epsilon \lambda(T^{+}) \nabla \theta \right]. \tag{5}$$

Because of the next two equations

$$\lim_{\epsilon \to 0} \frac{\rho c(T^+) - \rho c(T)}{\epsilon} = \frac{\partial \rho c}{\partial T} \theta, \tag{6}$$

$$\lim_{\epsilon \to 0} \frac{\lambda(T^+) - \lambda(T)}{\epsilon} = \frac{\partial \lambda}{\partial T} \theta, \tag{7}$$

divide ϵ on both sides of Eq.5 and let ϵ goes to 0. We have

$$\begin{split} \frac{\partial \rho c(T)}{\partial T} \theta \frac{\partial T}{\partial t} + \rho c(T) \frac{\partial \theta}{\partial t} &= \nabla \left[\frac{\partial \lambda}{\partial T} \theta \nabla T + \lambda(T) \nabla \theta \right] \\ \frac{\rho c(T)}{\partial t} \theta + \rho c(T) \frac{\partial \theta}{\partial t} &= \nabla \left(\theta \frac{\partial \lambda}{\partial T} \nabla T \right) + \nabla \lambda(T) \nabla \theta \\ \frac{\partial \rho c(T) \theta}{\partial t} &= \nabla^2 \left(\lambda(T) \theta \right). \end{split} \tag{8}$$

Next, from Eq.42(b), we have

$$T^{+}(\boldsymbol{x},0) = Y^{\xi}$$
$$T(\boldsymbol{x},0) = Y^{\xi}.$$

It is easy to get

$$\theta(\boldsymbol{x},0) = 0. \tag{9}$$

At last, we will derive the boundary conditions of the sensitivity problem. From Eq.42(c), we can get

$$\lambda(T^{+})\nabla T^{+} \cdot \boldsymbol{n} = q_{u} + \epsilon \Delta q_{u},$$
$$\lambda(T)\nabla T \cdot \boldsymbol{n} = q_{u}.$$

Subtract them and we have

$$\left[\lambda(T^{+})\nabla T^{+} - \lambda(T)\nabla T\right] \cdot \boldsymbol{n} = \epsilon \Delta q_{u}$$
$$\left[\lambda(T^{+})\nabla T + \lambda(T^{+})\epsilon \nabla \theta - \lambda(T)\nabla T\right] \cdot \boldsymbol{n} = \epsilon \Delta q_{u}.$$

Divide ϵ on both sides of the equation above and let ϵ goes to 0. Then, we have

$$\left[\frac{\partial \lambda}{\partial T}\theta \nabla T + \lambda(T)\nabla \theta\right] \cdot \boldsymbol{n} = \Delta q_u$$

$$\nabla \left(\lambda(T)\theta\right) \cdot \boldsymbol{n} = \Delta q_u. \tag{10}$$

Notice that, Eq.10 is satisfied on boundary Γ_u .

Similarly, we can also get

$$\nabla \left(\lambda(T)\theta \right) \cdot \boldsymbol{n} = 0 \tag{11}$$

on boundary Γ_g .

With Eq.8, Eq.9, Eq.10 and Eq.11, we can define the sensitivity problem

$$\begin{cases}
\rho \frac{\partial (c(T)\theta)}{\partial t} = \nabla^2 (\lambda(T)\theta) & (\boldsymbol{x},t) \in (\Omega, \mathcal{T}) \quad (a) \\
\theta(\boldsymbol{x},t;q_u, \Delta q_u) = 0 & \boldsymbol{x} \in \Omega \quad (b) \\
\nabla (\lambda(T)\theta) \cdot \boldsymbol{n} = \Delta q_u(\boldsymbol{x},t) & (\boldsymbol{x},t) \in (\Gamma_u, \mathcal{T}) \quad (c) \\
\nabla (\lambda(T)\theta) \cdot \boldsymbol{n} = 0 & (\boldsymbol{x},t) \in (\Gamma_g, \mathcal{T}) \quad (d)
\end{cases} \tag{12}$$

1.4 Dual Problem

Now, let's derive the dual problem. From Eq.12(a), we can get

$$\rho \frac{\partial \left(c(T)\theta \right)}{\partial t} - \nabla^2 \left(\lambda(T)\theta \right) = 0.$$

Multiply both sides of the equation above by ϕ and integrate on spatial domain Ω and time domain \mathcal{T}

$$\begin{split} 0 &= \int_{0}^{t_{f}} \int_{\Omega} \left[\rho \frac{\partial \left(c(T)\theta \right)}{\partial t} - \nabla^{2} \left(\lambda(T)\theta \right) \right] \phi d\Omega dt \\ &= \int_{\Omega} \int_{0}^{t_{f}} \rho \phi d \left(c(T)\theta \right) d\Omega - \int_{0}^{t_{f}} \int_{\partial \Omega} \nabla \left(\lambda(T)\theta \right) \cdot \boldsymbol{n} \phi d\Gamma dt + \int_{0}^{t_{f}} \int_{\Omega} \nabla \left(\lambda(T)\theta \right) \nabla \phi d\Omega dt \\ &= \int_{\Omega} \rho \phi c(T)\theta \Big|_{0}^{t_{f}} d\Omega - \int_{0}^{t_{f}} \int_{\Omega} \rho c(T)\theta \frac{\partial \phi}{\partial t} d\Omega dt - \int_{0}^{t_{f}} \int_{\partial \Omega} \nabla \left(\lambda(T)\theta \right) \cdot \boldsymbol{n} \phi d\Gamma dt + \int_{0}^{t_{f}} \int_{\Omega} \nabla \left(\lambda(T)\theta \right) \nabla \phi d\Omega dt \\ &= \int_{\Omega} \rho \phi c(T)\theta \Big|_{t_{f}} d\Omega - \int_{0}^{t_{f}} \int_{\Gamma_{u}} \nabla \left(\lambda(T)\theta \right) \cdot \boldsymbol{n} \phi d\Gamma dt + \int_{0}^{t_{f}} \int_{\Omega} \nabla \left(\lambda(T)\theta \right) \nabla \phi d\Omega dt - \int_{0}^{t_{f}} \int_{\Omega} \rho c(T)\theta \frac{\partial \phi}{\partial t} d\Omega dt \\ &= \int_{\Omega} \rho \phi c(T)\theta \Big|_{t_{f}} d\Omega - \int_{0}^{t_{f}} \int_{\Gamma_{u}} \nabla \left(\lambda(T)\theta \right) \cdot \boldsymbol{n} \phi d\Gamma dt - \int_{0}^{t_{f}} \int_{\Omega} \nabla^{2} \phi \left(\lambda(T)\theta \right) d\Omega dt \\ &+ \int_{0}^{t_{f}} \int_{\partial \Omega} \nabla \phi \cdot \boldsymbol{n} \left(\lambda(T)\theta \right) d\Omega dt - \int_{0}^{t_{f}} \int_{\Omega} \rho c(T)\theta \frac{\partial \phi}{\partial t} d\Omega dt \\ &= \int_{\Omega} \rho c(T)\theta \phi \Big|_{t_{f}} d\Omega - \int_{0}^{t_{f}} \int_{\Gamma_{u}} \Delta q_{u} \phi d\Gamma dt - \int_{0}^{t_{f}} \int_{\Omega} \left[\rho c(T) \frac{\partial \phi}{\partial t} + \lambda(T) \nabla^{2} \phi \right] \theta d\Omega dt \\ &+ \int_{0}^{t_{f}} \int_{\Gamma_{u}} \lambda(T) \nabla \phi \cdot \boldsymbol{n} \theta d\Omega dt + \int_{0}^{t_{f}} \int_{\Gamma_{g}} \lambda(T) \nabla \phi \cdot \boldsymbol{n} \theta d\Omega dt. \end{split} \tag{13}$$

From the definition of Eq.42, we can get

$$\mathcal{J}(q_u + \epsilon \Delta q_u) - \mathcal{J}(q_u) = \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} \left(T + \epsilon \theta - Y^{\xi} \right)^2 d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} \left(q_u + \epsilon \Delta q_u \right)^2 d\Gamma dt \\
- \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} \left(T - Y^{\xi} \right)^2 d\Gamma dt - \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} \left(q_u \right)^2 d\Gamma dt \\
= \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} \left(2\epsilon \theta T - 2\epsilon \theta Y^{\xi} + \epsilon^2 \theta^2 \right) d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} \left(2\epsilon q_u \Delta q_u + \epsilon^2 \Delta q_u^2 \right) d\Gamma dt$$

Then

$$(\mathcal{J}(q_u), \Delta q_u) = \lim_{\epsilon \to 0} \frac{\mathcal{J}(q_u + \epsilon \Delta q_u) - \mathcal{J}(q_u)}{\epsilon}$$

$$= \int_0^{t_f} \int_{\Gamma_u} \theta \left(T - Y^{\xi} \right) d\Gamma dt + \gamma \int_0^{t_f} \int_{\Gamma_u} q_u \Delta q_u d\Gamma dt$$
(14)

Based on Eq.14 and Eq.13, we can get the dual problem

$$\begin{cases}
\rho c(T) \frac{\partial \phi}{\partial t} = -\lambda(T) \nabla^2 \phi & (\boldsymbol{x}, t) \in (\Omega, \mathcal{T}) \quad (a) \\
\phi(\boldsymbol{x}, t_{\text{max}}) = 0 & \boldsymbol{x} \in \Omega \quad (b) \\
\lambda(T) \nabla \phi \cdot \boldsymbol{n} = 0 & (\boldsymbol{x}, t) \in (\Gamma_u, \mathcal{T}) \quad (c) \\
\lambda(T) \nabla \phi \cdot \boldsymbol{n} = T(\boldsymbol{x}, t; q_u) - Y^{\xi} \quad (\boldsymbol{x}, t) \in (\Gamma_g, \mathcal{T}) \quad (d)
\end{cases} \tag{15}$$

1.5 Derivative of Objective Function

Multiply both sides of Eq.12(a) by ϕ and integrate on Ω

$$\int_{0}^{t_{f}} \int_{\Omega} \rho \frac{\partial \left(c(T)\theta\right)}{\partial t} \phi d\Gamma dt = \int_{0}^{t_{f}} \int_{\Omega} \nabla \cdot \nabla \left(\lambda(T)\theta\right) \phi d\Gamma dt. \tag{16}$$

Left hand side of Eq.16 is

$$LHS = \int_{\Omega} \int_{0}^{t_{f}} \rho \phi d\left(c(T)\right) d\Omega$$

$$= \int_{\Omega} \left[\rho \phi c(T) \theta \Big|_{0}^{t_{f}} - \int_{0}^{t_{f}} \rho c(T) \theta \frac{\partial \phi}{\partial t} dt \right] d\Omega$$

$$= \int_{\Omega} \int_{0}^{t_{f}} \lambda(T) \nabla^{2} \phi \theta dt d\Omega$$

$$= \int_{0}^{t_{f}} \int_{\partial \Omega} \lambda(T) \nabla \phi \cdot \mathbf{n} \theta d\Gamma dt - \int_{0}^{t_{f}} \int_{\Omega} \nabla \left(\lambda(T) \theta\right) \nabla \phi d\Omega dt$$

$$= \int_{0}^{t_{f}} \int_{\Gamma_{a}} \lambda(T) \nabla \phi \cdot \mathbf{n} \theta d\Gamma dt - \int_{0}^{t_{f}} \int_{\Omega} \nabla \left(\lambda(T) \theta\right) \nabla \phi d\Omega dt. \tag{17}$$

In Eq.17, the third equality comes from Eq.12(b) and Eq.15(b) and the last equality comes from Eq.15(c). Right hand side of Eq.16 is

$$RHS = \int_{0}^{t_{f}} \int_{\partial\Omega} \nabla \left(\lambda(T)\theta\right) \cdot \boldsymbol{n}\phi d\Omega dt - \int_{0}^{t_{f}} \int_{\Omega} \nabla \left(\lambda(T)\theta\right) \nabla \phi d\Omega dt$$
$$= \int_{0}^{t_{f}} \int_{\Gamma_{u}} \nabla \left(\lambda(T)\theta\right) \cdot \boldsymbol{n}\phi d\Omega dt - \int_{0}^{t_{f}} \int_{\Omega} \nabla \left(\lambda(T)\theta\right) \nabla \phi d\Omega dt \tag{18}$$

The second equality of Eq.18 comes from Eq.12(d). Combine Eq.17 and Eq.18, we can get

$$\int_0^{t_f} \int_{\Gamma_q} \lambda(T) \nabla \phi \cdot \boldsymbol{n} \theta d\Omega dt = \int_0^{t_f} \int_{\Gamma_u} \nabla \left(\lambda(T) \theta \right) \cdot \boldsymbol{n} \phi d\Omega dt.$$

With Eq.12(c) and Eq.15(d), the equation above becomes

$$\int_{0}^{t_f} \int_{\Gamma_q} \left(T - Y^{\xi} \right) \theta d\Omega dt = \int_{0}^{t_f} \int_{\Gamma_u} \Delta q_u \phi d\Omega dt. \tag{19}$$

Combining Eq.14 and Eq.19, here comes

$$(\mathcal{J}(q_u), \Delta q_u) = \int_0^{t_f} \int_{\Gamma_g} \theta \left(T - Y^{\xi} \right) d\Gamma dt + \gamma \int_0^{t_f} \int_{\Gamma_u} q_u \Delta q_u d\Gamma dt$$

$$= \int_0^{t_f} \int_{\Gamma_u} \phi \Delta q_u d\Gamma dt + \gamma \int_0^{t_f} \int_{\Gamma_u} q_u \Delta q_u d\Gamma dt$$

$$= \int_0^{t_f} \int_{\Gamma_u} (\phi + \gamma q_u) \Delta q_u d\Gamma dt. \tag{20}$$

So it proves that Eq.21

$$\mathcal{J}'(q_u) = \phi + \gamma q_u. \tag{21}$$

1.6 Optimal Step Size

The expression for the optimal step size α_k is

$$\alpha_k = -\frac{\int_0^{t_f} \int_{\Gamma_g} \left(T_k - Y^{\xi} \right) \theta_k d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Gamma_u} \Delta q_{u,k} q_{u,k} d\Gamma dt}{\int_0^{t_f} \int_{\Gamma_g} \theta_k^2 d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Gamma_u} \Delta q_{u,k}^2 d\Gamma dt}.$$
(22)

In Eq.4, we replace ϵ with α , then

$$\mathcal{J}(q_{u,k+1}) = \mathcal{J}(q_{u,k} + \alpha_k \Delta q_{u,k})
= \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_{k+1} - Y^{\xi})^2 d\Gamma dt + \frac{\gamma_{k+1}}{2} \int_0^{t_f} \int_{\Gamma_u} (q_{u,k+1})^2 d\Gamma dt
= \frac{1}{2} \int_0^{t_f} T_k^2 + \alpha_k^2 \theta_k^2 + (Y^{\xi})^2 - 2T_k Y^{\xi} - 2\alpha_k \theta_k Y^{\xi} + 2T_k \alpha_k \theta_k d\Gamma dt
+ \frac{\gamma_{k+1}}{2} \int_0^{t_f} \int_{\Gamma_u} q_{u,k}^2 + \alpha_k^2 \Delta q_{u,k}^2 + 2\alpha_k q_{u,k} \Delta q_{u,k} d\Gamma dt$$

Taking derivative of $\mathcal{J}(q_{u,k+1})$ with α_k , we have

$$\frac{\partial \mathcal{J}(q_{u,k+1})}{\partial \alpha_k} = \int_0^{t_f} \int_{\Gamma_g} \alpha_k \theta_k^2 - \theta_k Y^{\xi} + \theta_k T_k d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Gamma_u} \alpha_k \Delta q_{u,k}^2 + q_{u,k} \Delta q_{u,k} d\Gamma dt. \quad (23)$$

Let Eq.23 equals to 0 and we can get Eq.22.

2 FEM with Adjoint Method for Solving Multi-layers Inverse Heat Conduction Problem

2.1 Primal Problem

We study on a multi-layers inverse heat condution problem which is defined on the domain showed in Fig.1. The heat flux on boundary Γ_g is known while it on Γ_u is unknown. $\Gamma_{ci}(i=1,2,\ldots,N-1)$

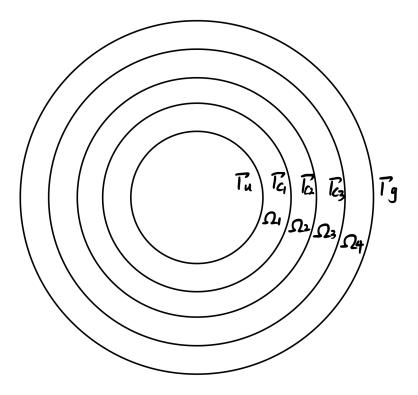


Figure 1: domain of the multi-layers heat conduction problem

is the interface of subdomain Ω_i and Ω_{i+1} .

The primal problem is discribed as below

$$\begin{cases}
\rho_{i}c_{i}(T_{i})\frac{\partial T_{i}}{\partial t} = \nabla \cdot (\lambda_{i}(T_{i})\nabla T_{i}) & (\boldsymbol{x},t) \in (\Omega_{i},\mathcal{T}) & (a) \\
T_{i}(\boldsymbol{x},0) = T_{i0} & \boldsymbol{x} \in \Omega_{i} & (b) \\
\lambda_{1}(T_{1})\nabla T_{1} \cdot \boldsymbol{n} = q_{u}(\boldsymbol{x},t) & (\boldsymbol{x},t) \in (\Gamma_{u},\mathcal{T}) & (c) \\
\lambda_{N}(T_{N})\nabla T_{N} \cdot \boldsymbol{n} = q_{g}(\boldsymbol{x},t) & (\boldsymbol{x},t) \in (\Gamma_{g},\mathcal{T}) & (d) \\
T_{i}(\boldsymbol{x},t) = T_{i+1}(\boldsymbol{x},t) & (\boldsymbol{x},t) \in (\Gamma_{i},\mathcal{T}) & (e) \\
\lambda_{i}(T_{i})\nabla T_{i} \cdot \boldsymbol{n}_{i} + \lambda_{i+1}(T_{i+1})\nabla T_{i+1} \cdot \boldsymbol{n}_{i+1} = 0 & (\boldsymbol{x},t) \in (\Gamma_{i},\mathcal{T}) & (f)
\end{cases}$$
(24)

where i = 1, 2, ..., N. To inverse the unknown heat flux on boundary Γ_u . We can set sensors on boundary Γ_g to detect the temperature distribution Y on it.

2.2 Object Function

The object function is

$$\mathcal{J}(q_u) = \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_N - Y)^2 d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} q_u^2 d\Gamma dt.$$
 (25)

Firstly, define

$$\theta_i = \lim_{\epsilon \to 0} \frac{T_i(q_u + \epsilon \Delta q_u) - T_i(q_u)}{\epsilon}.$$
 (26)

So

$$T_i(q_u + \epsilon \Delta q_u) \approx T_i(q_u) + \epsilon \theta_i.$$
 (27)

For simplicity, we note $T_i(q_u + \epsilon \Delta q_u)$ as T_i^+ and $T_i(q_u)$ as T_i . Then from Eq.25,

$$\lim_{\epsilon \to 0} \frac{\mathcal{J}(q_u + \epsilon \Delta q_u) - \mathcal{J}(q_u)}{\epsilon} = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left[\frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_N^+ - Y)^2 d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} (q_u + \epsilon \Delta q_u)^2 d\Gamma dt \right.$$

$$\left. - \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_N - Y)^2 d\Gamma dt - \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} q_u^2 d\Gamma dt \right]$$

$$= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left[\frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_N + \epsilon \theta_N - Y)^2 d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} (q_u + \epsilon \Delta q_u)^2 d\Gamma dt \right.$$

$$\left. - \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_N - Y)^2 d\Gamma dt - \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} q_u^2 d\Gamma dt \right]$$

$$= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left[\frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} \epsilon^2 \theta_N^2 + 2\epsilon \theta_N (T_N - Y) d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Gamma_u} \epsilon^2 \Delta q_u^2 + 2\epsilon q_u \Delta q_u d\Gamma dt \right]$$

$$= \int_0^{t_f} \int_{\Gamma_g} \theta_N (T_N - Y) d\Gamma dt + \gamma \int_0^{t_f} \int_{\Gamma_u} q_u \Delta q_u d\Gamma dt. \tag{28}$$

We take the note that

$$(\mathcal{J}'(q_u), \Delta q_u) := \int_0^{t_f} \int_{\Gamma_g} \theta_N(T_N - Y) d\Gamma dt + \gamma \int_0^{t_f} \int_{\Gamma_u} q_u \Delta q_u d\Gamma dt.$$
 (29)

2.3 Sensitivity Problem

From Eq.24(a), we have

$$\rho_i c_i(T_i^+) \frac{\partial T_i^+}{\partial t} = \nabla \cdot \left(\lambda_i(T_i^+) \nabla T_i^+ \right),$$
$$\rho_i c_i(T_i) \frac{\partial T_i}{\partial t} = \nabla \cdot \left(\lambda_i(T_i) \nabla T_i \right).$$

Then,

$$\rho_{i}c_{i}(T_{i}^{+})\frac{\partial T_{i}^{+}}{\partial t} - \rho_{i}c_{i}(T_{i})\frac{\partial T_{i}}{\partial t} = \nabla \cdot \left(\lambda_{i}(T_{i}^{+})\nabla T_{i}^{+} - \lambda_{i}(T_{i})\nabla T_{i}\right)$$

$$\rho_{i}c_{i}(T_{i}^{+})\frac{\partial T_{i}}{\partial t} + \rho_{i}c_{i}(T_{i}^{+})\epsilon\frac{\partial \theta_{i}}{\partial t} - \rho_{i}c_{i}(T_{i})\frac{\partial T_{i}}{\partial t} = \nabla \cdot \left(\lambda_{i}(T_{i}^{+})\nabla T_{i} + \lambda_{i}(T_{i}^{+})\epsilon\nabla\theta_{i} - \lambda_{i}(T_{i})\nabla T_{i}\right).$$

Deviding ϵ on both sides and let $\epsilon \to 0$, we have

$$\lim_{\epsilon \to 0} \frac{\rho_{i}c_{i}(T_{i}^{+}) - \rho_{i}c_{i}(T_{i})}{\epsilon} \frac{\partial T_{i}}{\partial t} + \rho_{i}c_{i}(T_{i}^{+}) \frac{\partial \theta_{i}}{\partial t} = \nabla \cdot \left(\lim_{\epsilon \to 0} \frac{\lambda_{i}(T_{i}^{+}) - \lambda_{i}(T_{i})}{\epsilon} \nabla T_{i} + \lambda_{i}(T_{i}^{+}) \nabla \theta_{i}\right)
\frac{\partial \rho_{i}c_{i}(T_{i})}{\partial T_{i}} \theta_{i} \frac{\partial T_{i}}{\partial t} + \rho_{i}c_{i}(T_{i}) \frac{\partial \theta_{i}}{\partial t} = \nabla \cdot \left(\frac{\partial \lambda_{i}(T_{i})}{\partial T_{i}} \theta_{i} \nabla T_{i} + \lambda_{i}(T_{i}) \nabla \theta_{i}\right)
\rho_{i} \frac{\partial c_{i}(T_{i})\theta_{i}}{\partial t} = \nabla \cdot (\nabla \lambda_{i}(T_{i})\theta_{i}).$$
(30)

From Eq.24(b), we have

$$T_i^+(t=0) - T_i(t=0) = T_{i0} - T_{i0}.$$

It is easy to get that

$$\theta_i(t=0) = 0. (31)$$

Then, on Γ_u , based on Eq.24(c)

$$(\lambda_1(T_1^+)\nabla T_1^+ - \lambda_1(T_1)\nabla T_1) \cdot \boldsymbol{n} = q_u + \epsilon \Delta q_u - q_u$$

$$(\lambda_1(T_1^+)\nabla T_1 + \epsilon \lambda_1(T_1^+)\nabla \theta_1 - \lambda_1(T_1)\nabla T_1) \cdot \boldsymbol{n} = \epsilon \Delta q_u.$$

Deviding ϵ on both sides and let $\epsilon \to 0$

$$\lim_{\epsilon \to 0} \left(\frac{\lambda_1(T_1^+) - \lambda_1(T_1)}{\epsilon} \nabla T_1 + \lambda_1(T_1^+) \nabla \theta_1 \right) \cdot \boldsymbol{n} = \delta q_u$$

$$\left(\frac{\partial \lambda_1(T_1)}{\partial T_1} \theta_1 \nabla T_1 + \lambda_1(T_1) \nabla \theta_1 \right) \cdot \boldsymbol{n} = \Delta q_u$$

$$\nabla \left(\lambda_1(T_1) \theta_1 \right) \cdot \boldsymbol{n} = \Delta q_u. \tag{32}$$

Similarly, we can get

$$\nabla \left(\lambda_N(T_N)\theta_N \right) \cdot \boldsymbol{n} = 0 \tag{33}$$

on Γ_q .

Next, from Eq.24(e), we can get

$$T_i^+ - T_i = T_{i+1}^+ - T_{i+1}$$

$$\epsilon \theta_i = \epsilon \theta_{i+1}$$

$$\theta_i = \theta_{i+1}$$
(34)

on Γ_i .

At last, from Eq.24(f),

$$\left(\lambda_i(T_i^+)\nabla T_i^+ - \lambda_i(T_i)\nabla T_i\right) \cdot \boldsymbol{n}_i + \left(\lambda_{i+1}(T_{i+1}^+)\nabla T_{i+1}^+ - \lambda_{i+1}(T_{i+1})\nabla T_{i+1}\right) \cdot \boldsymbol{n}_{i+1} = 0.$$

It is easy to derive that

$$\nabla(\lambda_i(T_i)\theta_i) \cdot \boldsymbol{n}_i + \nabla(\lambda_{i+1}(T_{i+1})\nabla\theta_{i+1}) \cdot \boldsymbol{n}_{i+1} = 0.$$
(35)

Combining Eq.30, Eq.31, Eq.32, Eq.33, Eq.34 and Eq.35, we have the sensitivity problem

$$\begin{cases}
\rho_{i} \frac{\partial c_{i}(T_{i})\theta_{i}}{\partial t} = \nabla \cdot (\nabla \lambda_{i}(T_{i})\theta_{i}) & (\boldsymbol{x},t) \in (\Omega_{i},\mathcal{T}) & (a) \\
\theta_{i}(t=0) = 0 & \boldsymbol{x} \in \Omega_{i} & (b) \\
\nabla (\lambda_{1}(T_{1})\theta_{1}) \cdot \boldsymbol{n} = \Delta q_{u} & (\boldsymbol{x},t) \in (\Gamma_{u},\mathcal{T}) & (c) \\
\nabla (\lambda_{N}(T_{N})\theta_{N}) \cdot \boldsymbol{n} = 0 & (\boldsymbol{x},t) \in (\Gamma_{g},\mathcal{T}) & (d) \\
\theta_{i} = \theta_{i+1} & (\boldsymbol{x},t) \in (\Gamma_{i},\mathcal{T}) & (e) \\
\nabla (\lambda_{i}(T_{i})\theta_{i}) \cdot \boldsymbol{n}_{i} + \nabla (\lambda_{i+1}(T_{i+1})\nabla \theta_{i+1}) \cdot \boldsymbol{n}_{i+1} = 0 & (\boldsymbol{x},t) \in (\Gamma_{i},\mathcal{T}) & (f)
\end{cases}$$
(36)

where i = 1, 2, ..., N.

2.4 Dual Problem

According to Eq.36(a), one can get

$$0 = \sum_{i=1}^{N} \int_{0}^{t_f} \int_{\Omega_i} \left(\rho_i \frac{\partial c_i(T_i)\theta_i}{\partial t} - \nabla \cdot (\nabla \lambda_i(T_i)\theta_i) \right) \phi_i d\Omega dt.$$

Then,

$$\begin{split} 0 &= \sum_{i=1}^{N} \left(\int_{0}^{t_f} \int_{\Omega_i} \rho_i \frac{\partial c_i(T_i)\theta_i}{\partial t} \phi_i d\Omega dt - \int_{0}^{t_f} \int_{\Omega_i} \nabla \cdot \left(\nabla \lambda_i(T_i)\theta_i \right) \phi_i d\Omega dt \right) \\ &= \sum_{i=1}^{N} \left(\int_{\Omega_i} \int_{0}^{t_f} \rho_i \phi_i d\left(c_i(T_i)\theta_i \right) d\Omega - \int_{0}^{t_f} \int_{\Omega_i} \nabla \cdot \left(\nabla \lambda_i(T_i)\theta_i \right) \phi_i d\Omega dt \right) \\ &= \sum_{i=1}^{N} \left(\int_{\Omega_i} \rho_i c_i(T_i)\theta_i \phi_i \Big|_{0}^{t_f} d\Omega - \int_{0}^{t_f} \int_{\Omega_i} \rho_i c_i(T_i)\theta_i \frac{\partial \phi_i}{\partial t} d\Omega dt \right. \\ &- \int_{0}^{t_f} \int_{\partial \Omega_i} \nabla \lambda_i(T_i)\theta_i \cdot \boldsymbol{n} \phi_i d\Gamma dt + \int_{0}^{t_f} \int_{\Omega_i} \nabla \lambda_i(T_i)\theta_i \nabla \phi_i d\Omega dt \right) \\ &= \sum_{i=1}^{N} \left(\int_{\Omega_i} \rho_i c_i(T_i)\theta_i \phi_i \Big|_{t_f} d\Omega - \int_{0}^{t_f} \int_{\Omega_i} \rho_i c_i(T_i)\theta_i \frac{\partial \phi_i}{\partial t} d\Omega dt \right. \\ &- \int_{0}^{t_f} \int_{\partial \Omega_i} \nabla \lambda_i(T_i)\theta_i \cdot \boldsymbol{n} \phi_i d\Gamma dt + \int_{0}^{t_f} \int_{\partial \Omega_i} \lambda_i(T_i)\theta_i \nabla \phi_i \cdot \boldsymbol{n} d\Gamma dt \\ &- \int_{0}^{t_f} \int_{\Omega_i} \lambda_i(T_i)\theta_i \nabla \cdot \nabla \phi_i d\Omega dt \right) \end{split}$$

$$\begin{split} &= \sum_{i=1}^{N} \bigg(\int_{\Omega_{i}} \rho_{i} c_{i}(T_{i}) \theta_{i} \phi_{i} \big|_{t_{f}} d\Omega - \int_{0}^{t_{f}} \int_{\Omega_{i}} \Big(\rho_{i} c_{i}(T_{i}) \frac{\partial \phi_{i}}{\partial t} + \lambda_{i}(T_{i}) \nabla \cdot \nabla \phi_{i} \Big) \theta_{i} d\Omega dt \\ &- \Big(\int_{0}^{t_{f}} \int_{\Gamma_{g}} \nabla \lambda_{N}(T_{N}) \theta_{N} \cdot \mathbf{n} \phi_{N} d\Gamma dt + \int_{0}^{t_{f}} \int_{\Gamma_{u}} \nabla \lambda_{1}(T_{1}) \theta_{1} \cdot \mathbf{n} \phi_{1} d\Gamma dt \\ &+ \int_{0}^{t_{f}} \int_{\Gamma_{i}} \nabla \lambda_{i}(T_{i}) \theta_{i} \cdot \mathbf{n} \phi_{i} + \nabla \lambda_{i+1}(T_{i+1}) \theta_{i+1} \cdot \mathbf{n} \phi_{i+1} d\Gamma dt \Big) \\ &+ \Big(\int_{0}^{t_{f}} \int_{\Gamma_{g}} \lambda_{N}(T_{N}) \theta_{N} \nabla \phi_{N} \cdot \mathbf{n} d\Gamma dt + \int_{0}^{t_{f}} \int_{\Gamma_{u}} \lambda_{1}(T_{1}) \theta_{1} \nabla \phi_{1} \cdot \mathbf{n} d\Gamma dt \\ &+ \int_{0}^{t_{f}} \int_{\Gamma_{i}} \lambda_{i}(T_{i}) \theta_{i} \nabla \phi_{i} \cdot \mathbf{n} + \lambda_{i+1}(T_{i+1}) \theta_{i+1} \nabla \phi_{i+1} \cdot \mathbf{n} d\Gamma dt \Big) \Big) \\ &= \sum_{i=1}^{N} \bigg(\int_{\Omega_{i}} \rho_{i} c_{i}(T_{i}) \theta_{i} \phi_{i} \big|_{t_{f}} d\Omega - \int_{0}^{t_{f}} \int_{\Omega_{i}} \Big(\rho_{i} c_{i}(T_{i}) \frac{\partial \phi_{i}}{\partial t} + \lambda_{i}(T_{i}) \nabla \cdot \nabla \phi_{i} \Big) \theta_{i} d\Omega dt \\ &- \Big(\int_{0}^{t_{f}} \int_{\Gamma_{u}} \Delta q_{u} \phi_{1} d\Gamma dt + \int_{0}^{t_{f}} \int_{\Gamma_{i}} \nabla \lambda_{i}(T_{i}) \theta_{i} \cdot \mathbf{n} \phi_{i} + \nabla \lambda_{i+1}(T_{i+1}) \theta_{i+1} \cdot \mathbf{n} \phi_{i+1} d\Gamma dt \Big) \\ &+ \Big(\int_{0}^{t_{f}} \int_{\Gamma_{g}} \lambda_{N}(T_{N}) \theta_{N} \nabla \phi_{N} \cdot \mathbf{n} d\Gamma dt + \int_{0}^{t_{f}} \int_{\Gamma_{u}} \lambda_{1}(T_{1}) \theta_{1} \nabla \phi_{1} \cdot \mathbf{n} d\Gamma dt \\ &+ \int_{0}^{t_{f}} \int_{\Gamma_{i}} \lambda_{i}(T_{i}) \theta_{i} \nabla \phi_{i} \cdot \mathbf{n} + \lambda_{i+1}(T_{i+1}) \theta_{i+1} \nabla \phi_{i+1} \cdot \mathbf{n} d\Gamma dt \Big) \Big). \end{aligned} \tag{37}$$

On the basis of Eq.36, dual problem is raised as below

$$\begin{cases}
\rho_{i}c_{i}(T_{i})\frac{\partial\phi_{i}}{\partial t} = -\lambda_{i}(T_{i})\nabla \cdot \nabla\phi_{i} & (\boldsymbol{x},t) \in (\Omega_{i},\mathcal{T}) & (a) \\
\phi_{i}(t=t_{f}) = 0 & \boldsymbol{x} \in \Omega_{i} & (b) \\
\lambda_{1}(T_{1})\nabla\phi_{1} \cdot \boldsymbol{n} = 0 & (\boldsymbol{x},t) \in (\Gamma_{u},\mathcal{T}) & (c) \\
\lambda_{N}(T_{N})\nabla\phi_{N} \cdot \boldsymbol{n} = T_{N} - Y & (\boldsymbol{x},t) \in (\Gamma_{g},\mathcal{T}) & (d) \\
\phi_{i} = \phi_{i+1} & (\boldsymbol{x},t) \in (\Gamma_{i},\mathcal{T}) & (e) \\
\lambda_{i}(T_{i})\nabla\phi_{i} \cdot \boldsymbol{n}_{i} + \lambda_{i+1}(T_{i+1})\nabla\phi_{i+1} \cdot \boldsymbol{n}_{i+1} = 0 & (\boldsymbol{x},t) \in (\Gamma_{i},\mathcal{T}) & (f)
\end{cases}$$
(38)

where i = 1, 2, ..., N.

So Eq.37 can be written as

$$0 = -\int_0^{t_f} \int_{\Gamma_u} \Delta q_u \phi_1 d\Gamma dt + \int_0^{t_f} \int_{\Gamma_g} \theta_N (T_N - Y) d\Gamma dt.$$
 (39)

Then, combine Eq.29 and Eq.39, we can get the derivative of object function $\mathcal{J}(q_u)$ is

$$\mathcal{J}'(q_u) = \phi_1 + \gamma q_u. \tag{40}$$

2.5 Optimal Step Size

Replacing ϵ with α_k , then

$$\begin{split} \mathcal{J}(q_{u,k+1}) = & \mathcal{J}(q_{u,k} + \alpha_k \Delta q_{u,k}) \\ = & \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_{N,k+1} - Y)^2 d\Gamma dt + \frac{\gamma_{k+1}}{2} \int_0^{t_f} \int_{\Gamma_u} (q_{u,k+1})^2 d\Gamma dt \\ = & \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_{N,k} + \alpha_k \theta_{N,k} - Y)^2 d\Gamma dt + \frac{\gamma_{k+1}}{2} \int_0^{t_f} \int_{\Gamma_u} (q_{u,k} + \alpha_k \Delta q_{u,k})^2 d\Gamma dt \\ = & \frac{1}{2} \int_0^{t_f} \int_{\Gamma_g} (T_{N,k} - Y)^2 + \alpha_k^2 \theta_{N,k}^2 + 2\alpha_k \theta_{N,k} (T_{N,k} - Y) d\Gamma dt \\ & + \frac{\gamma_{k+1}}{2} \int_0^{t_f} \int_{\Gamma} q_{u,k}^2 + \alpha_k^2 \Delta q_{u,k}^2 + 2\alpha_k q_{u,k} \Delta q_{u,k} d\Gamma dt \end{split}$$

Taking derivative of $\mathcal{J}(q_{u,k+1})$ with α_k

$$\frac{\partial \mathcal{J}(q_{u,k+1})}{\partial \alpha_k} = \int_0^{t_f} \int_{\Gamma_q} \alpha_k \theta_{N,k}^2 + \theta_{N,k} (T_{N,k} - Y) d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Gamma_u} \alpha_k \Delta q_{u,k}^2 + q_{u,k} \Delta q_{u,k} d\Gamma dt.$$

Letting $\partial \mathcal{J}(q_{u,k+1})/\partial \alpha_k$ equals to 0, then we can get the optimal step

$$\alpha_k = -\frac{\int_0^{t_f} \int_{\Gamma_g} (T_{N,k} - Y) \theta_{N,k} d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Gamma_u} q_{u,k} \Delta q_{u,k} d\Gamma dt}{\int_0^{t_f} \int_{\Gamma_g} \theta_{N,k}^2 d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Gamma_u} \Delta q_{u,k}^2 d\Gamma dt}.$$
(41)

3 An Iterative Finite-Element Algorithm for Solving Nonlinear Inverse Heat Conduction Problems With Unknown Conduction Coefficient

In this problem, the coefficient of heat conduction $\lambda(T)$ is unknown. Then we consider λ is function of \boldsymbol{x} and t which is $\lambda(\boldsymbol{x},t)$.

3.1 Primal Problem

$$\begin{cases}
\rho c(T) \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) & (\boldsymbol{x}, t) \in (\Omega, \mathcal{T}) \quad \text{(a)} \\
T(\boldsymbol{x}, 0) = \tilde{Y}^{\xi} & \boldsymbol{x} \in \Omega \quad \text{(b)} \\
\lambda \nabla T \cdot \boldsymbol{n} = q(\boldsymbol{x}, t) & (\boldsymbol{x}, t) \in (\partial \Omega, \mathcal{T}) \quad \text{(c)}
\end{cases}$$

3.2 Objective Function

From the primal problem, we define the objective function

$$\mathcal{J}(\lambda) = \frac{1}{2} \int_0^{t_f} \int_{\partial\Omega} \left(T - Y^{\xi} \right)^2 d\Gamma dt + \frac{\gamma}{2} \int_0^{t_f} \int_{\Omega} \lambda^2 d\Omega dt. \tag{43}$$

3.3 Sensitivity Problem

First

$$\theta(\boldsymbol{x}, t; \lambda, \Delta \lambda) = \lim_{\epsilon \to 0} \frac{T(\boldsymbol{x}, t; \lambda + \epsilon \Delta \lambda) - T(\boldsymbol{x}, t; \lambda)}{\epsilon}, \tag{44}$$

Then

$$T(\boldsymbol{x}, t; \lambda + \epsilon \Delta \lambda) \approx T(\boldsymbol{x}, t; \lambda) + \epsilon \theta(\boldsymbol{x}, t; \lambda, \Delta \lambda).$$
 (45)

Note that

$$T^+ := T(\lambda + \epsilon \Delta \lambda),$$

 $T := T(\lambda).$

From

$$\rho c(T^{+}) \frac{\partial T^{+}}{\partial t} - \rho c(T) \frac{\partial T}{\partial t} = \nabla \left((\lambda + \epsilon \Delta \lambda) \nabla T^{+} \right) - \nabla \left(\lambda \nabla T \right)$$
(46)

we can get

$$\rho c(T^{+}) \frac{\partial T}{\partial t} - \rho c(T) \frac{\partial T}{\partial t} + \epsilon \rho c(T^{+}) \frac{\partial \theta}{\partial t} = \nabla \left(\epsilon \Delta \lambda \nabla T + \epsilon \lambda \nabla \theta + \epsilon^{2} \Delta \lambda \nabla \theta \right)$$
(47)

Divide ϵ on both sides of equation above and let ϵ goes to 0. We have

$$\lim_{\epsilon \to 0} \frac{\rho c(T^{+}) - \rho c(T)}{\epsilon} \frac{\partial T}{\partial t} + \rho c(T) \frac{\partial \theta}{\partial t} = \nabla \cdot (\Delta \lambda \nabla T + \lambda \nabla \theta)$$
$$\frac{\partial \rho c(T)}{\partial T} \theta \frac{\partial T}{\partial t} + \rho c(T) \frac{\partial \theta}{\partial t} = \nabla \cdot (\Delta \lambda \nabla T + \lambda \nabla \theta)$$

It is easy to get

$$\theta(\boldsymbol{x},0) = 0. \tag{48}$$

$$(\lambda + \epsilon \Delta \lambda) \nabla T^{+} \cdot \mathbf{n} = q,$$

$$\lambda \nabla T \cdot \mathbf{n} = q.$$
 (49)

$$(\epsilon \Delta \lambda \nabla T + \epsilon \lambda \nabla \theta + \epsilon^2 \Delta \lambda \nabla \theta) \cdot \mathbf{n} = 0$$

$$(\Delta \lambda \nabla T + \lambda \nabla \theta) \cdot \mathbf{n} = 0$$
(50)

So, the sensitivity problem is

$$\begin{cases}
\frac{\partial \rho c(T)\theta}{\partial t} = \nabla \cdot (\lambda \nabla \theta + \Delta \lambda \nabla T) & (\boldsymbol{x}, t) \in (\Omega, \mathcal{T}) \\
\theta(\boldsymbol{x}, 0) = 0 & \boldsymbol{x} \in \Omega & (b) \\
(\lambda \nabla \theta + \Delta \lambda \nabla T) \cdot \boldsymbol{n} = 0 & (\boldsymbol{x}, t) \in (\partial \Omega, \mathcal{T}) & (c)
\end{cases}$$
(51)

3.4 Dual Problem

Based on the first equation of sensitivity problem

$$\begin{split} 0 &= \int_0^{t_f} \int_\Omega \left[\rho \frac{\partial c(T)\theta}{\partial t} - \nabla \cdot (\lambda \nabla \theta + \Delta \lambda \nabla T) \right] \phi d\Omega dt \\ &= \int_\Omega \rho \phi d \left(c(T)\theta \right) d\Omega - \int_0^{t_f} \int_{\partial\Omega} \left(\Delta \lambda \nabla T + \lambda \nabla \theta \right) \cdot \boldsymbol{n} \phi d\Gamma dt + \int_0^{t_f} \int_\Omega \left(\Delta \lambda \nabla T + \lambda \nabla \theta \right) \nabla \phi d\Omega dt \\ &= \int_\Omega \rho \phi c(T)\theta \big|_0^{t_f} d\Omega - \int_0^{t_f} \int_\Omega \rho c(T)\theta \frac{\partial \phi}{\partial t} d\Omega dt + \int_0^{t_f} \int_\Omega \Delta \lambda \nabla T \nabla \phi d\Omega dt + \int_0^{t_f} \int_\Omega \lambda \nabla \theta \nabla \phi d\Omega dt \\ &= \int_\Omega \rho \phi c(T)\theta \big|_{t_f} d\Omega + \int_0^{t_f} \int_\Omega \Delta \lambda \nabla T \nabla \phi d\Omega dt + \int_0^{t_f} \int_{\partial\Omega} \nabla \phi \cdot \boldsymbol{n} (\lambda \theta) d\Gamma dt - \int_0^{t_f} \int_\Omega \nabla^2 \phi \lambda \theta d\Omega dt \\ &= \int_\Omega \rho \phi c(T)\theta \big|_{t_f} d\Omega + \int_0^{t_f} \int_\Omega \Delta \lambda \nabla T \nabla \phi d\Omega dt + \int_0^{t_f} \int_{\partial\Omega} \lambda \nabla \phi \cdot \boldsymbol{n} \theta d\Gamma dt - \int_0^{t_f} \int_\Omega \left(\rho c(T) \frac{\partial \phi}{\partial t} + \lambda \nabla^2 \phi \right) \theta d\Omega dt \\ &= \int_\Omega \rho \phi c(T)\theta \big|_{t_f} d\Omega + \int_0^{t_f} \int_\Omega \Delta \lambda \nabla T \nabla \phi d\Omega dt + \int_0^{t_f} \int_{\partial\Omega} \lambda \nabla \phi \cdot \boldsymbol{n} \theta d\Gamma dt - \int_0^{t_f} \int_\Omega \left(\rho c(T) \frac{\partial \phi}{\partial t} + \lambda \nabla^2 \phi \right) \theta d\Omega dt \end{split}$$

According to object function, we can get

$$\mathcal{J}(\lambda + \epsilon \Delta \lambda) - \mathcal{J}(\lambda) = \frac{1}{2} \int_{0}^{t_f} \int_{\partial \Omega} \left(T + \epsilon \theta - Y^{\xi} \right)^{2} d\Gamma dt + \frac{\gamma}{2} \int_{0}^{t_f} \int_{\Omega} (\lambda + \epsilon \Delta \lambda)^{2} d\Omega dt
- \frac{1}{2} \int_{0}^{t_f} \int_{\partial \Omega} \left(T - Y^{\xi} \right)^{2} d\Gamma dt - \frac{\gamma}{2} \int_{0}^{t_f} \int_{\Omega} \lambda^{2} d\Omega dt
= \frac{1}{2} \int_{0}^{t_f} \int_{\partial \Omega} \left(2\epsilon \theta T - 2\epsilon \theta Y^{\xi} + \epsilon^{2} \theta^{2} \right) d\Gamma dt + \frac{\gamma}{2} \int_{0}^{t_f} \int_{\Omega} \left(2\epsilon \lambda \Delta \lambda + \epsilon^{2} \Delta \lambda^{2} \right) d\Omega dt \tag{52}$$

Divide ϵ on both sides of the eqution above and we can get

$$\lim_{\epsilon \to 0} \frac{\mathcal{J}(\lambda + \epsilon \Delta \lambda) - \mathcal{J}(\lambda)}{\epsilon} = \int_{0}^{t_f} \int_{\partial \Omega} \theta \left(T - Y^{\xi} \right) d\Gamma dt + \gamma \int_{0}^{t_f} \int_{\Omega} \lambda \Delta \lambda d\Omega dt \tag{53}$$

So dual problem is

$$\begin{cases}
\rho c(T) \frac{\partial \phi}{\partial t} = -\lambda \nabla^2 \phi & (\boldsymbol{x}, t) \in (\Omega, \mathcal{T}) & (a) \\
\phi(\boldsymbol{x}, t_f) = 0 & x \in \Omega & (b) \\
\lambda \nabla \phi \cdot \boldsymbol{n} = T - Y^{\xi} & (\boldsymbol{x}, t) \in (\partial \Omega, \mathcal{T}) & (c)
\end{cases} \tag{54}$$

Let α_k represents ϵ and p_k represents $\Delta \lambda$. Then we get

$$\alpha_k = -\frac{\int_0^{t_f} \int_{\partial\Omega} \left(T_k - Y^{\xi} \right) \theta_k d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Omega} \lambda_k p_k d\Omega dt}{\int_0^{t_f} \int_{\partial\Omega} \theta_k^2 d\Gamma dt + \gamma_{k+1} \int_0^{t_f} \int_{\Omega} p_k^2 d\Omega dt}$$
(55)

$$\beta_k = \begin{cases} 0\\ \max(0, \beta^{PR}) \end{cases} \tag{56}$$

$$\beta^{PR} = \frac{\int_0^{t_f} \int_{\Omega} \mathcal{J}'(\lambda_k) \left[\mathcal{J}'(\lambda_k) - \mathcal{J}'(\lambda_{k-1}) \right] d\Omega dt}{\int_0^{t_f} \int_{\Omega} \left[\mathcal{J}'(\lambda_{k-1}) \right]^2 d\Omega dt}$$
(57)

$$p_k = \begin{cases} -\mathcal{J}'(\lambda_k) \\ -\mathcal{J}'(\lambda_k) + \beta_k p_{k-1} \end{cases}$$
 (58)

And the derivative of object function is

$$\mathcal{J}'(\lambda) = \nabla T \nabla \phi - \gamma \lambda \tag{59}$$

3.5 Discretization of One Dimensional Primal Problem

$$\begin{cases}
\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \lambda \frac{\partial T}{\partial x} \\
T(x,0) = Y^{\xi} \\
-\lambda \frac{\partial T}{\partial x}(0,t) = q_{1}(t) \\
\lambda \frac{\partial T}{\partial x}(1,t) = q_{2}(t)
\end{cases} (60)$$

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{(\lambda_{i+1}^n + \lambda_i^n) T_{i+1}^n - (\lambda_{i+1}^n + 2\lambda_i^n + \lambda_{i-1}^n) T_i^n + (\lambda_i^n + \lambda_{i-1}^n) T_{i-1}^n}{4\Delta x^2} + \frac{(\lambda_{i+1}^{n+1} + \lambda_i^{n+1}) T_{i+1}^{n+1} - (\lambda_{i+1}^{n+1} + 2\lambda_i^{n+1} + \lambda_{i-1}^{n+1}) T_i^{n+1} + (\lambda_i^{n+1} + \lambda_{i-1}^{n+1}) T_{i-1}^{n+1}}{4\Delta x^2}$$
(61)

$$+\frac{(\lambda_{i+1}^{n+1}+\lambda_{i}^{n+1})T_{i+1}^{n+1}-(\lambda_{i+1}^{n+1}+2\lambda_{i}^{n+1}+\lambda_{i-1}^{n+1})T_{i}^{n+1}+(\lambda_{i}^{n+1}+\lambda_{i-1}^{n+1})T_{i-1}^{n+1}}{4\Delta x^{2}} \quad (62)$$

3.6 Discretization of One Dimensional Dual Problem

$$\begin{cases}
\frac{\partial \phi}{\partial t} = -\lambda \nabla^2 \phi \\
\phi(x, t_f) = 0 \\
\lambda \nabla \phi \cdot \mathbf{n} = T - Y^{\xi}
\end{cases}$$
(63)

It is clear that dual problem is a backward problem which has a 'final condition'. Let $t = t_f - \tau$ and we can get a forward problem.

$$\begin{cases}
\frac{\partial \phi}{\partial \tau} = \lambda \nabla^2 \phi \\
\phi(x,0) = 0 \\
\lambda \nabla \phi \cdot \mathbf{n} = T - Y^{\xi}
\end{cases}$$
(64)

Discretization of One Dimensional Sensitivity Problem 3.7

$$\begin{cases}
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial \theta}{\partial x} + \Delta \lambda \frac{\partial T}{\partial x} \right) \\
\theta(x,0) = 0 \\
\lambda \frac{\partial \theta}{\partial x}(0,t) + \Delta \lambda \frac{\partial T}{\partial x}(0,t) = 0 \\
\lambda \frac{\partial \theta}{\partial x}(1,t) + \Delta \lambda \frac{\partial T}{\partial x}(1,t) = 0
\end{cases}$$
(65)

Calcuate $\Delta \lambda$ (p_k) 3.7.1

$$p_k = \begin{cases} -\mathcal{J}'(\lambda_k) \\ -\mathcal{J}'(\lambda_k) + \beta_k p_{k-1} \end{cases}$$
 (66)

3.7.2 Discretization

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial \theta}{\partial x} + p \frac{\partial T}{\partial x} \right) \tag{67}$$

$$\begin{split} \frac{\theta_i^{n+1} - \theta_i^n}{\Delta t} &= \frac{(\lambda_{i+1}^n + \lambda_i^n)\theta_{i+1}^n - (\lambda_{i+1}^n + 2\lambda_i^n + \lambda_{i-1}^n)\theta_i^n + (\lambda_i^n + \lambda_{i-1}^n)\theta_{i-1}^n}{4\Delta x^2} \\ &\quad + \frac{(\lambda_{i+1}^{n+1} + \lambda_i^{n+1})\theta_{i+1}^{n+1} - (\lambda_{i+1}^{n+1} + 2\lambda_i^{n+1} + \lambda_{i-1}^{n+1})\theta_i^{n+1} + (\lambda_i^{n+1} + \lambda_{i-1}^{n+1})\theta_{i-1}^{n+1}}{4\Delta x^2} \\ &\quad + \frac{(p_{i+1}^n + p_i^n)T_{i+1}^n - (p_{i+1}^n + 2p_i^n + p_{i-1}^n)T_i^n + (p_i^n + p_{i-1}^n)T_{i-1}^n}{4\Delta x^2} \\ &\quad + \frac{(p_{i+1}^{n+1} + p_i^{n+1})T_{i+1}^{n+1} - (p_{i+1}^{n+1} + 2p_i^{n+1} + p_{i-1}^{n+1})T_i^{n+1} + (p_i^{n+1} + p_{i-1}^{n+1})T_{i-1}^{n+1}}{4\Delta x^2} \end{split}$$