Application of Fitzpatrick Sequences to Solve a Heat Transfer Problem

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ABSTRACT
The purpose of the article is to resolve the heat equation by optimizing a functional. Various cases of thermal conductivity tensors are developed. The Legendre-Fenchel-Moreau convex transformation is particularly used. Using the Fitzpatrick method, appropriate increasing sequences are built for materials with linear but asymmetric heat transfer.

Keywords
Heat transfer, Variational principle, Legendre-Fenchel transform, Fitzpatrick's series, Functional optimization

1. INTRODUCTION
Since the goal of this study is to resolve the heat equation through a functional optimization. The first step is to look for a variational principle in the linear case of the thermal conductivity tensor , homogeneous or not, but symmetric. Next, the study is extended to the nonlinear case in which the thermal conductivity tensor is not symmetric. In particular, the focus is on the Legendre-Fenchel-Moreau convex transformation that provides a systematic procedure to introduce duality into convex optimisation problems. Using the Fitzpatrick's method, an appropriate increasing sequence is built in the case in which the operator is not cyclically monotonic but only n-monotonic.

2. POSITION OF THE PROBLEM
The boundary value problem oftransient heat conduction is established by expressing the solid thermal equilibium, introducing the Fourier law connecting the heat flux to the temperature gradient and formulating boundary conditions. Thus, this problem is expressed as[1]:

$$\begin{cases} \text{Find } \theta(x,y,t) \text{ at any point } M(x,y)\in\Omega \text{ verifying:} \\ \text{at } t=0:\ \theta(x,y,0)=\theta_0(x,y) \\ \text{at any instant } t\in\left]0,t_f\right[: \\ \rho c\dfrac{d\theta}{dt}=div\left(-\Lambda.grad\theta\right)+Q \quad \text{in } \Omega \\ h=D\phi\left(grad\,\theta\right) \quad \text{in } \Omega \\ \left.\begin{array}{l}\left(-\Lambda.grad\theta\right).n=q \quad \text{on } \Gamma_q \\ \quad\theta=\theta_d \quad \text{on } \Gamma_\theta\end{array}\right\} \text{ with } \Gamma_q\cup\Gamma_\theta=\Gamma \end{cases} \tag{1}$$

Where :
$\theta(x,y,t)$ is the temperature at point $M(x,y)$ of the body Ω at a time *t*, Q is the heat source, $h=\Lambda.grad\theta$ is the opposite of the heat flux density vector, ρ is the density, *c* is the specific heat of the mass and $\Lambda=\begin{pmatrix}\lambda_{11} & \lambda_{12}\\ \lambda_{21} & \lambda_{22}\end{pmatrix}$ the thermal conductivity tensor homogeneous or not but its symmetrical part is defined positive. *D* is the derivative operator.

The boundary conditions are represented on body's boundary Γ by a known flux density $h.n=q$ applied on a part Γ_q of Γ and by a known temperature $\theta=\theta_d$ on the complementary part Γ_θ .

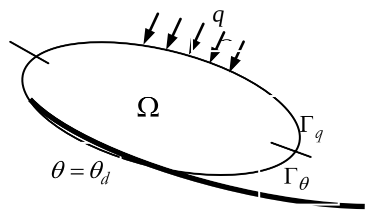

Figure 1: The body Ω

The solving of the problem leads to the minimization of the following functional:

$$\begin{aligned} F(\theta,h)=&\int_\Omega\left(\phi\left(grad\,\theta\right)+\phi^*\left(h\right)\right)dS+\int_\Omega\theta\left[\rho c\frac{d\theta}{dt}\right]dS \\ &-\int_\Omega Q\theta dS-\int_{\Gamma_\theta}\theta_d h.n\,d\ell-\int_{\Gamma_q}q\theta\,d\ell \end{aligned} \tag{2}$$

$\phi\left(grad\,\theta\right)=\frac{1}{2}\left(\Lambda\,grad\,\theta\right).grad\,\theta$ is a scalar function that is both convex and differentiable, called a potential, and $\phi^*\left(h\right)$ is it's conjugate potential which represents the Legendre-Fenchel-Moreau transform of the function [2].

Since the Fenchel's inequality reads:

$$\phi\left(grad\,\theta\right)+\phi^*\left(h\right)\geq h.grad\,\theta \tag{3}$$

And using the Stokes and the following tensor formulas:

$$h.grad\,\theta=\text{div}\left(\theta h\right)-\theta div\left(h\right) \tag{4}$$

The problem of minimization becomes:

$$\begin{aligned} F(\theta,h)\geq&\int_{\Gamma_q}\theta\left(h.n-q\right)d\ell+\int_{\Gamma_\theta}(\theta-\theta_d)h.n\,d\ell \\ &-\int_\Omega\theta\left[div\,h+Q-\rho c\frac{d\theta}{dt}\right]dS=0 \end{aligned} \tag{5}$$

Among the θ and *h*satisfying:

$$\begin{cases} div(h)+Q=\rho c\dfrac{d\theta}{dt} \\ h.n=q \;\; sur \;\; \Gamma_q \qquad in\ \Omega\times\left]0,t_f\right[\\ \theta=\theta_d \;\; sur \;\; \Gamma_\theta \\ \theta(x,y,0)=\theta_0(x,y) \end{cases} \quad (6)$$

F is a positive convex functional. The equality of F to zero occurs when the Fenchel's inequality reduces to the equality:

$$\phi(grad\,\theta)+\phi^*(h)=h.grad\,\theta \qquad (7)$$

That is, when the constitutive law is satisfied in the form: $h=D\phi(grad\,\theta)$ or in the conjugate form: $grad\,\theta=D\phi^*(h)$.

The minimization of the functional F which is globally convex allows to solve our problem. Numerically, the Uzawa's method is appropriate, it alternates iteratively between improvements in θ and h fields.

3. CASE WHERE Λ IS SYMMETRIC

If the tensor Λ is symmetric and positive definite, it is said that the material belongs to the class of Generalized Standard Materials (G.S.M.) [3]. It can be characterized by the convex potential: $\phi(grad\,\theta)=\frac{1}{2}(\Lambda\,grad\,\theta).grad\,\theta$. Its inverse law is characterized by the conjugate convex potential: $\phi^*(h)=\frac{1}{2}(h\Lambda^{-1}h)$. Its behaviour is described by one of the three following laws:

$$\begin{cases} grad\,\theta\in\partial\phi^*(h) \\ h\in\partial\phi(grad\,\theta) \\ \phi(grad\,\theta)+\phi^*(h)=h.grad\,\theta \end{cases} \qquad (8)$$

Where the symbol ∂ denotes the sub-differential.

In this case there is a variational principle in order to find $grad\,\theta$ directly (**primal method**) and a variational principle in order to find h directly (**dual method**).

3.1. Primal method

Actually, a primal method is possible to determine θ directly by minimizing the functional G:

$$G(\theta)=\int_\Omega \phi(grad\,\theta)dS+\int_\Omega \theta\left[\rho c\frac{d\theta}{dt}-Q\right]dS-\int_{\Gamma_q}\theta q d\ell \quad (9)$$

Among the θ satisfying: $\theta=\theta_d$ on Γ_θ.

Indeed, for all $\delta\theta$ null on Γ_θ:

$$\delta G(\theta)=\int_\Omega \big(D\phi(grad\,\theta)grad\,\delta\theta\big)dS+\int_\Omega \theta\left[\rho c\left(\frac{d\delta\theta}{dt}\right)\right]dS$$
$$+\int_\Omega \delta\theta\left[\rho c\frac{d\theta}{dt}-Q\right]dS-\int_{\Gamma_q}\delta\theta q d\ell$$

$\delta\theta$ can be seen as a virtual temperature at fixed time t according to the virtual work principle, then : $\dfrac{d\delta\theta}{dt}=0$

Hence:

$$\delta G(\theta)=\int_\Omega div\big(\delta\theta D\phi(grad\,\theta)\big)dS-\int_\Omega \delta\theta div\big(D\phi(grad\,\theta)\big)dS$$
$$+\int_\Omega \delta\theta\left[\rho c\frac{d\theta}{dt}-Q\right]dS-\int_{\Gamma_q}\delta\theta q d\ell$$

$$\delta G(\theta)=\int_{\Gamma_q}\delta\theta\big(n.D\phi(grad\,\theta)-q\big)d\ell+\int_{\Gamma_\theta}\delta\theta\big(n.D\phi(grad\,\theta)\big)d\ell$$
$$-\int_\Omega \delta\theta div\big(D\phi(grad\,\theta)\big)dS+\int_\Omega \delta\theta\left[\rho c\frac{d\theta}{dt}-Q\right]dS=0$$

(10)

3.2. Dual method

Once θ is determined, a dual method is possible to determine h by minimizing the functional H:

$$H(h)=\int_\Omega \phi^*(h)dS-\int_{\Gamma_\theta}\theta_d\,h.n\,d\ell \qquad (11)$$

Among the h satisfying:

$$\begin{cases} div(h)+Q=\rho c\dfrac{d\theta}{dt} \\ h.n=q \;\; on \;\; \Gamma_q \qquad in\ \Omega\times\left]0,t_f\right[\\ \theta=\theta_d \;\; on \;\; \Gamma_\theta \end{cases} \qquad (12)$$

By introducing a Lagrange multiplier $-\theta$ to account for the $div(\delta h)$:

$$\delta H(h)=\int_\Omega D\phi^*(h).\delta h\,dS-\int_{\Gamma_\theta}\theta_d\,\delta h.n\,d\ell=\int_\Omega -\theta.div(\delta h)dS$$
$$=\int_\Omega\big(-div(\theta\delta h)+\delta h\,grad\,\theta\big)dS$$
$$=-\int_{\Gamma_\theta}\theta\delta h\ .n\,d\ell\ +\int_\Omega \delta h\ .grad\,\theta\,dS \qquad (13)$$

Since the study is restricted to $div(h)+Q=\rho c\dfrac{d\theta}{dt}$ in Ω and $h.n=q$ on Γ_q, the PDEis resolved and θ is interpreted as the solution of the primal problem. Once h is determined numerically, the field $grad\,\theta$ is determined as well. And as $\theta=\theta_d$ on Γ_θ, the field θ is also determined.

4. CASE WHERE Λ IS NOT SYMMETRIC

In the case of Λ is not symmetric but h is related to the temperature gradient by a constitutive law of the type:

$$h=D\phi(grad\,\theta) \quad \text{with } \phi \text{ convex} \qquad (14)$$

The graphs of the operators of such constitutive laws are cyclically monotonic.

As in mechanical engineering in which those operators are applied to Generalized Standard Materials (GSM), the multivalued operatorscan even been accepted.

The functions ϕ and ϕ^* are then only convex and *lower semi-continuous*.

The constitutive law is then expressed as a sub-differential inclusion:

$$h\in\delta_\theta\phi(grad\,\theta\,,h) \qquad (15)$$

Or equivalently by:

$$grad\,\theta \in \delta_h \phi^*\left(grad\,\theta\,,h\right) \qquad (16)$$

The two-field variational principle persists because it is based on the equivalence of these two sub-differential inclusions with the scalar condition: $\phi\left(grad\,\theta\right)+\phi^*\left(h\right)=h.grad\,\theta$ as underlined by J.J. Moreau. More generally, the sum $\phi\left(grad\,\theta\right)+\phi^*\left(h\right)$ is replacedby a biconvex function called the bipotential $b\left(h,grad\,\theta\right)$.

Materials whose constitutive law can be represented by a bipotential are called Implicit Standard Materials (I.S.M.)[4].

Hence, the solution of the problem leads to the minimization of the following functional:

$$F\left(\theta,h\right)=\int_\Omega b\left(h,grad\,\theta\right)dS-\int_\Omega \theta\left[\rho c\frac{d\theta}{dt}-Q\right]dS$$
$$-\int_{\Gamma_\theta}\theta_d h.n\,d\ell-\int_{\Gamma_q}\theta h.n\,d\ell \qquad (17)$$

However, it may happen that the graph of the operator relating the flux vector h to the gradient vector $grad\,\theta$ is only k-monotonic (k finite). Is there, in this case, a variational principle to solve the problem.

5. FITZPATRICK FUNCTION FOR ALINEAR LAW

In order to solve problem,the bipotential $b\left(h,grad\,\theta\right)$ is replaced by a Fitzpatrick sequence $F_{\lambda,n}\left(h,grad\theta\right)$ in the functional $F\left(\theta,h\right)$ [5,6].

The functional to be minimized is then:

$$F\left(\theta,h\right)=\int_\Omega F_{\lambda,n}\left(h,grad\theta\right)dS-\int_\Omega \theta\left[\rho c\frac{d\theta}{dt}-Q\right]dS$$
$$-\int_{\Gamma_\theta}\theta_d h.n\,d\ell-\int_{\Gamma_q}\theta h.n\,d\ell \qquad (18)$$

The construction of the Fitzpatrick sequence for the $h=\Lambda grad\theta$ is possible if the single-valued operator Λ is monotonic.

In the case where the monotonicity condition is reduced to the positive definition of the symmetric part S of Λ, the expression of the sequence is:

$$F_{\lambda,n}\left(h,grad\theta\right)=tr\left(grad\theta,h\right)$$
$$+\frac{1}{4}tr\left(h-\Lambda grad\theta,H_{n-2}^{-1}\left(h-\Lambda grad\theta\right)\right) \qquad (19)$$

$$\begin{cases} H_n=S-\dfrac{1}{4}\Lambda^t H_{n-1}^{-1}\Lambda \\ H_0=S=\begin{pmatrix}\lambda_{11} & \left(\lambda_{12}+\lambda_{21}\right)/2\\ \left(\lambda_{12}+\lambda_{21}\right)/2 & \lambda_{22}\end{pmatrix}\end{cases}$$

The tensor Λ is then splitted: $\Lambda=S+\dfrac{\lambda_{12}+\lambda_{21}}{2}J$, such that : $J=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$. So, $\Lambda^T=S-\dfrac{\lambda_{12}+\lambda_{21}}{2}J$.

Introducing the decompositions of Λ^T and Λ and knowing that for 2x2 symmetric invertible matrices: $J\,S^{-1}J=\dfrac{-S}{\det S}$, then:

$$H_1=\left(1-\frac{1}{4}\left(1+\left(\frac{\lambda_{12}+\lambda_{21}}{2}\right)^2\frac{1}{\det S}\right)\right)S$$

And H_1 is proportional to *S*. Therefore:

$$H_0=\frac{\xi_0}{2}S \quad \text{with } \xi_0=2$$

$$H_1=\frac{\xi_1}{2}S \;\text{ with } \xi_1=2-\frac{1}{\xi_0}\left(1+\left(\frac{\lambda_{12}+\lambda_{21}}{2}\right)^2\frac{1}{\det S}\right)$$

Let us assume that $H_{i-1}=\dfrac{\xi_{i-1}}{2}S$ with

$$\xi_{i-1}=2-\frac{1}{\xi_{i-2}}\left(1+\left(\frac{\lambda_{12}+\lambda_{21}}{2}\right)^2\frac{1}{\det S}\right)$$

Let us show that $H_i=\dfrac{\xi_i}{2}S$

$$H_i=S-\left(S-\frac{\lambda_{12}+\lambda_{21}}{2}J\right)\frac{2}{\xi_{i-1}}S^{-1}\left(S+\frac{\lambda_{12}+\lambda_{21}}{2}J\right)$$
$$=\left(1-\frac{1}{2\xi_{i-1}}\left(1+\left(\frac{\lambda_{12}+\lambda_{21}}{2}\right)^2\frac{1}{\det S}\right)\right)S$$

Hence: $H_i=\dfrac{\xi_i}{2}S$ with $\xi_i=2-\dfrac{1}{\xi_{i-1}}\left(1+\left(\dfrac{\lambda_{12}+\lambda_{21}}{2}\right)^2\dfrac{1}{\det S}\right)$

The coefficient ξ_{n-2} is obtained by recursion.

Let us introduce a positive variable x defined by:

$$1+\left(\frac{\lambda_{12}+\lambda_{21}}{2}\right)^2\frac{1}{\det S}=\frac{1}{x^2}$$

We have $\det S=\lambda_{11}\lambda_{22}-\left(\dfrac{\lambda_{12}+\lambda_{21}}{2}\right)^2$

So: $X=\sqrt{1-\left(\dfrac{\lambda_{12}+\lambda_{21}}{2}\right)^2\dfrac{1}{\lambda_{11}\lambda_{22}}}$

The introduction of the variable *X* in the different terms of the sequence ξ_i leads to:

$$\xi_i=2-\frac{1}{\alpha_{i-1}X^2} \quad \text{and } \xi_i X=2X-\frac{1}{\xi_{i-1}X}$$

Afterwardsthe sequence $\psi_i=\xi_i X$ is studied preferably.

The sequence ψ_i begins by the following terms : $\psi_0=2X$, $\psi_1=2X-\dfrac{1}{\psi_0}$ and $\psi_i=2X-\dfrac{1}{\psi_{i-1}}=\xi_i X$.

The expression of ψ_i is introduced in a sequence of Chebychev's polynomials of second kind $P_i(X)$ in such a way that $P_0(X)=1$ and $P_1(X)=2X$, thus:

$$\psi_0=\frac{P_1(X)}{P_0(X)} \text{ and } \psi_1=2X-\frac{P_0(X)}{P_1(X)}=\frac{P_2(X)}{P_1(X)}$$

With $P_2(X)=2XP_1(X)-P_0(X)$.

From these two results, a recursion formula for ψ_i can be initiated. Let us suppose that $\psi_{i-1}=\frac{P_i(X)}{P_{i-1}(X)}$ with

$P_i(X)=2XP_{i-1}(X)-P_{i-2}(X)$.

Then, the next term of the sequence can be expressed as:

$$\psi_i = 2X - \frac{P_{i-1}(X)}{P_i(X)} = \frac{2XP_i(X)-P_{i-1}(X)}{P_i(X)} = \frac{P_{i+1}(X)}{P_i(X)}$$

Hence, the calculus of ψ_{n-2} can be achieved by recursion.

In the construction of the $P_i(X)$, the Chebychev's polynomials of the second kind is recognized.

Since X is less or equal 1, one can set $X=\cos\alpha$ with $0\le\alpha\le\pi/2$ and these polynomials become successively:

$$P_0(X)=1,\ P_1(x)=2\cos\alpha=\frac{\sin(2\alpha)}{\sin\alpha},$$

$$P_2(x)=4\cos^2\alpha-1=\frac{\sin(3\alpha)}{\sin\alpha},\ \dots,\ P_i(x)=\frac{\sin((i+1)\alpha)}{\sin\alpha}$$

This new formulation of Chebychev's polynomials leads to a new expression of the sequence ψ_i :

$$\psi_0=\frac{P_1(X)}{P_0(X)}=\frac{\sin 2\alpha}{\sin\alpha}\ ,\ \psi_1=\frac{P_2(X)}{P_1(X)}=\frac{\sin(3\alpha)}{\sin(2\alpha)},\ \dots,$$

$$\psi_i(x)=\frac{\sin((i+2)\alpha)}{\sin((i+1)\alpha)}.$$

Thus the sequence ξ_i :

$$\xi_0=\frac{\psi_0}{\cos\alpha}=2\ ,\ \xi_1=\frac{\sin(3\alpha)}{\sin(2\alpha).\cos\alpha},\ \dots,$$

$$\xi_i(x)=\frac{\sin((i+2)\alpha)}{\sin((i+1)\alpha).\cos\alpha}\ \text{ et }\ \xi_{n-2}(x)=\frac{\sin(n\alpha)}{\sin((n-1)\alpha).\cos\alpha}$$

The previous developments relative to H_i leads to conclude that:

$$H_{n-2}=\frac{\sin(n\alpha)}{2\sin((n-1)\alpha).\cos\alpha}S \text{ with}$$

$$\cos\alpha=\sqrt{1-\left(\frac{\lambda_{12}+\lambda_{21}}{2}\right)^2\frac{1}{\lambda_{11}\lambda_{22}}}$$

$$F_{\lambda,n}(h,grad\theta)=tr(grad\theta,h) + \frac{1}{4}tr\left(h-\Lambda grad\theta, H_{n-2}^{-1}(h-\Lambda grad\theta)\right)$$

Hence finally:

$$F_{\lambda,n}(grad\theta,h)=tr(grad\theta,h) + \frac{1}{4}tr\left(h-\Lambda grad\theta, H_{n-2}^{-1}(h-\Lambda grad\theta)\right)$$

$$= h.grad\theta + \frac{1}{2}(h-\Lambda grad\theta)\frac{\sin((n-1)\alpha).\cos\alpha}{\sin(n\alpha)}\ S^{-1}(h-\Lambda grad\theta)$$

$$= h.grad\theta + \frac{1}{2}\frac{\sin(n-1)\alpha\ \cos\alpha}{\sin n\alpha}(h-\Lambda grad\theta)\ S^{-1}(h-\Lambda grad\theta)$$

Hence, the functional to be minimized is written as:

$$F(\theta,h)=\int_\Omega\left[\begin{array}{l} h.grad\theta+\frac{1}{2}\frac{\sin(n-1)\alpha\ \cos\alpha}{\sin n\alpha}. \\ (h-\lambda grad\theta)\ S^{-1}(h-\lambda grad\theta)\end{array}\right]dS - \int_\Omega\theta\left[\rho c\frac{d\theta}{dt}\right]dS - \int_{\partial\Omega_q}\theta h.n\, d\ell \qquad (20)$$

The functional $F(\theta,h)$ is the sum of a function of $grad\theta$ and a function of h only if the coupling term $\frac{1}{2}\frac{\sin(n-1)\alpha\ \cos\alpha}{\sin n\alpha}(h-\lambda grad\theta)\ S^{-1}(h-\lambda grad\theta)$ is zero. This is only possible if Λ is symmetric, i.e. $\alpha=0$. When α is non-zero the Fitzpatrick sequence stops at $k=n$ for n finite.

6. CONCLUSION

The consideration of Fitzpatrick functions allows to extend energy methods to the solution of the heat transfer problem. An optimal bipotential for material for which thermal conductivity tensor is not isotropic is derived. By the same technique, other non-associated constitutive laws can be modelised.

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