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An inverse problem and diffusion limit for the phonon transport equation

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A parabolic type heat equation has long been used to model heat propagation. It was discovered recently that the underlying ab-initio model should be the phonon transport equation, a type of kinetic equation. When two materials are placed adjacent to each other, the heat that propagates from one to the other experiences thermal boundary resistance. Mathematically, this is represented by the reflection coefficient of the phonon transport equation at the interface of the two materials.

In the first part of this work, we formulate an inverse problem for the reconstruction of this reflection coefficient [1]. We employ maximum principle to show the well-posedness of the forward problem, formulate the inverse problem as a PDE-constrained minimization, and apply stochastic gradient descent to conduct the parameter reconstruction.

In the second part, we investigate the numerical implementation of the limiting equation for the phonon transport equation in the small Knudsen number regime [2]. In this regime, the phonon transport equation achieves the heat equation as its asymptotic limit in the interior, and forms a boundary layer at the physical boundary. The boundary layer can be represented by a Robin-type boundary condition for the heat equation, and we provide a numerical strategy for finding the Robin coefficients by solving an auxiliary half-space equation. More specifically, the half-space solver is composed of a spectral method that achieves spectral accuracy, with even-odd decomposition to eliminate corner singularities.

1 Model and inverse problem setup

In experiments, two solid materials, e.g. aluminium and silicon, are placed side by side, and heat is injected on the surface of one material. Temperature is also measured at the same location as a function of time [3]. Denote the location of the surface of aluminum to be $x = 0$ and the interface to be $x = 1$. The governing equation is the phonon transport equation, given by

$$
\begin{aligned}
&\partial_t g + \mu v(\omega)\partial_x g = \mathcal{L}g\,, \quad x \in [0,1] \\
&\quad g(x=0\,,\mu\,,\cdot) = \phi\,, \quad \mu > 0 \\
&\quad g(x=1\,,\mu\,,\cdot) = \eta(\omega) g(x=1\,,-\mu\,,\cdot)\,, \quad \mu < 0
\end{aligned}
$$

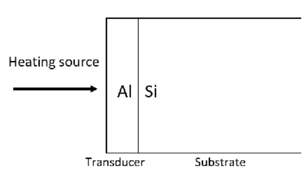

Figure 1: Experimental setup

with $\mathcal{L}g = \frac{-g}{\tau(\omega)} + \frac{\langle g/\tau\rangle}{\langle g^*/\tau\rangle} g^*(\omega)$, where the angle brackets denote integration with respect to μ and ω. $g(t,x,\mu,\omega)$ is the probability density of phonons at location x moving with velocity μ that oscillates at frequency ω, at time t and η is the reflection coefficient. $g^* = \partial_T F^*|_{T_0}$, where F^* is the equilibrium distribution in the form of $\frac{\hbar\omega D(\omega)}{e^{\hbar\omega/k_{\mathrm{B}}T}-1}$. From conservation laws, the change in temperature $\Delta T = \frac{\langle \omega g\rangle}{\langle \omega g^*\rangle}$. The temperature term T in the definition of F^* is determined to ensure the energy is conserved, in the sense that $\int \mathcal{L}g\, dv\, d\omega = 0$ for all (x,t). The goal is to infer the reflection index $\eta(\omega)$ using the measurements taken on the surface of the metal: ΔT. Let d_{ij} correspond to the measurement using source ϕ_i, with test function ψ_j. We can

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formulate the inverse problem as the following least squares minimization problem

$$\min_{\eta} \frac{1}{IJ} \sum_{i,j} |\mathcal{M}_{ij}(\eta) - d_{ij}|^2 = \min_{\eta} \frac{1}{IJ} \sum_{i,j} L_{i,j}^2 \tag{1}$$

where $\mathcal{M}_{ij}(\eta) = \int \Delta T_i(x = 0, t)\psi_j(t)dt$. Because of the summation structure of the loss function in (1), we choose to apply the SGD method. In [1], we also show maximum principle and Lipschitz continuiity of the Fréchet derivative to justify the use of SGD in this setup. As a numerical example, we choose $x \in [0, 0.5]$, $t \in [0, 5]$, $\mu \in [-1, 1]$, and $\omega \in [0.05, 2]$ and set the reference η as $\eta = (\tanh(10(\omega - 1.5)) - \tanh(2(\omega - 1)))/4 + 1/2$. For testing, we set $I = 40$ and $J = 1$ with $\phi_i = \delta(\omega - \omega_i)$ and $\psi_j = \delta(t - t_{\max})$.

2 Diffusion Limit

In order to study the diffusion limit of (1), we restrict ourselves to the steady state case:

$$\begin{cases} \mu \partial_x g & = \frac{1}{\mathsf{Kn}} (\mathcal{L}g - g) \\ g(x = 0, \mu, \omega) & = \phi, \quad \mu > 0 \\ g(x = 1, \mu, \omega) & = \eta(\omega) g(x = 1, -\mu, \omega), \quad \mu < 0 \end{cases} \tag{2}$$

where $\mathsf{Kn} = \mathsf{Kn}(\omega) = v\tau/L$ for some length scale L. When L is significantly larger than the average travel distance $\|\boldsymbol{v}_g\|\tau$, the Knudsen number Kn is small. In this case, one can derive the asymptotic limit of the phonon transport equation that characterizes its macroscopic behavior [2]. In the presence of non-trivial boundary conditions, there will be thin layers in both left and right physical boundaries of the domain, and the layers are of width $\langle \mathsf{Kn} \rangle$. To proceed, we will write the approximated solution as $g^{\mathrm{A}} = g^{\mathrm{L}} + g^{\mathrm{in}} + g^{\mathrm{R}}$ with the three terms taking care of the left boundary layer, interior solution and right boundary layer respectively. Here, the interior solution $g^{\mathrm{in}} = \rho - v\mathsf{Kn}\partial_x \rho$, with ρ satisfying the diffusion equation $\partial_{xx}\rho = 0$ with boundary conditions $b_1\rho - b_2\partial_x\rho = b_0$ at $x = 0$ and $b_3\rho + b_4\partial_x\rho = 0$ at $x = 1$. Here b_i are constants that can be solved for by matching the values of the left and right boundary layers, g^{L} and g^{R} to be zero near the right and left boundaries respectively. Details can be found in [2]. As a numerical example, consider a source function $\phi = \mu$ and reflection coefficient $\eta = (\tanh(10(\omega - 1.5)) - \tanh(2(\omega - 1)))/4 + 1/2$ with $\omega \in [0.4, 2.4]$.

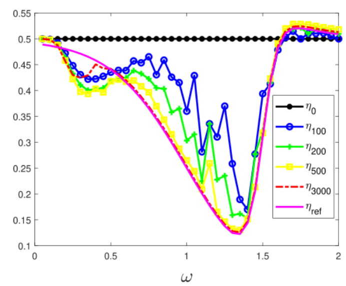

Figure 2: Inverse example: Profile of reflection coefficient at different iteration steps. The initial guess is $\eta_0 = 0.5$. The solution at n = 3000 almost recovers the reference solution.

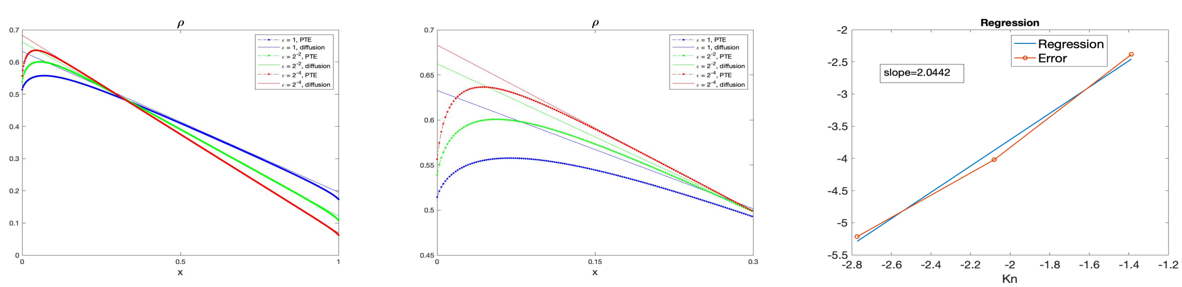

Figure 3: The panel on the left shows the density ρ over the whole domain. The panel in the middle shows the layer behavior close to $x = 0$ computed using different Kn and the limiting ρ. The panel on the right shows the convergence rate on the log-log scale. It suggests the asymptotic convergence is Kn^2. The incoming data is $\phi = v$ for the multiple frequency.

References

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