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Predicting subdifferential switching surface in a steady-state complex heat transfer problem using deep learning

A boundary value problem of complex heat transfer have been considered in the work. A method for determination of a switching surface with subdifferential boundary conditions based on the use of deep learning has been proposed. A method uses a neural network trained on a dataset of numerical solutions of the steady-state complex heat transfer forward problems. The obtained results are verified by comparison with the numerical experiments.

Key words: *Subdifferential boundary value problem, deep learning, neural networks, complex heat transfer.*

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Introduction

The search for new ways to solve complex heat transfer systems is relevant in connection with practical applications in combustion chambers [1] and in glass production [2]. The system consists of the heat equation and the integro-differential radiative transfer equation which, due to the complexity of the solution, is replaced by the P_1–approximation [3]. Solving complex heat transfer problems with boundaries which depend on external conditions are the most relevant due to practical applications.

The stationary radiative and conductive heat transfer problem is described by the system consisting of the heat transfer equation and P_1–approximation of the radiative transfer equation. The steady-state model of complex heat transfer in the bounded domain $\Omega \subset \mathbb{R}^2$ including the boundary conditions has the following form [4], [5]:

$$-a\Delta\theta + b\kappa_a(|\theta|\theta^3 - \varphi) = 0, \quad -\alpha\Delta\varphi + \kappa_a(\varphi - |\theta|\theta^3) = 0, \tag{1}$$

$$\partial_n\theta + \beta(\theta - \theta_b)|_\Gamma = 0, \quad \alpha\partial_n\varphi + \gamma(\varphi - \theta_b^4)|_\Gamma = 0, \tag{2}$$

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where θ is the normalized temperature, φ is the normalized intensity of radiation, averaged over all directions, κ_a is the absorption coefficient, ∂_n denotes the derivative in the direction of the outward normal $\mathbf{n}$ to the domain boundary $\Gamma = \partial\Omega$.

The coefficients a, b, α, β, γ are expressed as follows:

$$a = \frac{k}{\rho c_v}\left[\frac{\text{cm}^2}{\text{s}}\right], \quad b = \frac{4\sigma n^2 T_{max}^3}{\rho c_v}\left[\frac{\text{cm}}{\text{s}}\right], \quad \alpha = \frac{1}{3\kappa - A\kappa_s}\left[\frac{1}{\text{cm}}\right],$$
$$\beta = \frac{h}{\rho c_v}\left[\frac{\text{cm}}{\text{s}}\right], \quad \gamma = \frac{\epsilon}{2(2-\epsilon)},$$

where h is the heat transfer coefficient of the boundary domain [kg/(s^{3}K)], ϵ is the surface emissivity, k is the coefficient of thermal conductivity [kg $\cdot$ cm/s^{3}K], ρ is the density [kg/cm^3], c_v is the specific heat capacity [cm^2/s^{2}K], σ is the Stefan-Boltzmann constant [kg/s^{3}K^4], n is the refractive index, T_{max} is the maximum temperature in the non-normalized model [K], κ is the total attenuation factor [1/cm], κ_s is the scattering coefficient [1/cm], A is the scattering anisotropy coefficient, $A \in [-1; 1]$.

We assume that the parameter γ has the following form [6]:

$$\gamma(\varphi) = \begin{cases} \gamma_1, & \varphi > \theta_0^4, \\ [\gamma_1, \gamma_2], & \varphi = \theta_0^4, \\ \gamma_2, & \varphi < \theta_0^4, \end{cases} \tag{3}$$

where γ_1, γ_2, θ_0 are given functions, $0 \le \gamma_1 \le \gamma_2$, $0 \le \theta_0 \le \theta_b$. Then the boundary conditions (2) can be written in the following form [6]:

$$-\alpha\partial_n\varphi \in \partial g(\varphi), \quad g(\varphi) = \begin{cases} \dfrac{\gamma_0}{2}(\varphi - \theta_b^4)^2 & \text{if } \varphi \ge \theta_b^4, \\ \dfrac{\gamma_1}{2}(\varphi - \theta_b^4)^2 + \dfrac{\gamma_0 - \gamma_1}{2}(\theta_0^4 - \theta_b^4) & \text{if } \varphi < \theta_b^4, \end{cases} \tag{4}$$

where ∂g denotes the subdifferential of a convex function g.

The subdifferential boundary value problem (1)–(3) was studied in [6], where a priori estimates for the weak solution were obtained and the unique solvability of the problem was proved.

In systems employing "bang-bang" control law, which is used in (3), switching surface separates regions of maximum and minimum control efforts. The switching surface is defined by parameters P, γ_1 and γ_2, where P is the switching point, γ_1 and γ_2 are values of γ before and after switching. As soon as γ_1 and γ_2 are considered given, the goal of this work is to determine parameter P.

1 Numerical simulation and dataset generation

To solve the stationary forward problem of complex heat transfer (1)–(2), where $\gamma = const$, Newton's method is used. The conditions for the convergence of Newton's method are established in a similar way as in the proof of the uniqueness of a weak solution to the problem (1)–(2) [4]. When solving the forward problem with a switching surface defined by the functions P, γ_1 and γ_2, satisfying to the subdifferential boundary condition (3), we obtain a switching point P for given γ_1 and γ_2 if the method converges.

The problem is simulated numerically using FreeFEM++ software [7]. A square with the side length of L was chosen as the computational domain. The temperatures θ_b and θ_0 are chosen as follows:

$$\theta_b = F + \left(\frac{y}{BL}\right)^G, \quad \theta_0 = \theta_b,$$

where B, G, F are given parameters.

To solve the problem using machine learning, it is necessary to generate a dataset. The model parameters and their minimum and maximum values used in data generation are shown in Table 1. Thus, the physical characteristics of the medium and the boundary conditions vary. The variable ranges have been chosen to be as wide as possible to cover different problems. Dataset is generated according to the uniform distribution.

Table 1: Model parameters

Parameter	Minimum value	Maximum value	Units
ρ	$0.15 \cdot 10^{-6}$	$7500 \cdot 10^{-6}$	$\mathrm{kg/cm^3}$
c_v	$5 \cdot 10^6$	$52 \cdot 10^6$	$\mathrm{cm^2/s^2K}$
T_{max}	273	3000	K
n	1	2	–
k	0	6000	$\mathrm{kg \cdot cm/s^3K}$
κ	0.01	2	1/cm
κ_s	0	0.01	1/cm
A	-1	1	–
L	25	150	cm
γ_1	0.0	0.25	–
γ_2	0.25	0.5	–
h	0.1	500	$\mathrm{kg/(s^3K)}$
B	2.0	4.0	–
G	1.0	3.0	–
F	0.0	$1 - (1/B)^G$	–

2 Machine learning

To find the switching point, the supervised learning method is used. The selected model learns to find non-obvious statistical relationships between the input and the output data. The input data are the parameters presented in Table 1. The output data is the switching point P, i.e. the point where $\varphi = \theta_0^4$.

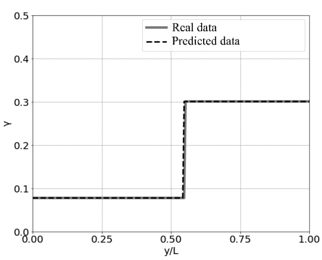
Standard metrics MAE (mean absolute error) and R^2 (coefficient of determination) are used to evaluate the prediction results of neural network:

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n} |y_i - x_i|, \quad \mathrm{R}^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - x_i)}{\sum_{i=1}^{n}(y_i - \overline{y})},$$

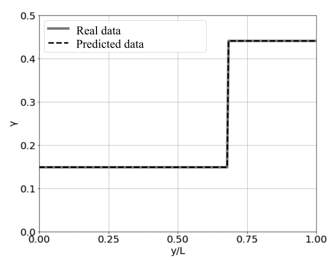
where y_i is the predicted value, x_i is the numerical simulation value and $\overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$.

The neural network was trained using generated dataset. A total of 16,000 experiments have been performed. The model was trained using 10-fold cross validation. The results are as follows: $\mathrm{R}^2 = 0.928$, MAE $= 2.02$. High R^2 value (close to unity) indicates a high quality of prediction. MAE indicates an error in absolute values, but since the value of the switch point is a percentage of the border size ($0{-}100\%$ of L), it can be considered the same as a percentage error. The error of 2% is a small deviation, which shows the high quality of prediction. Four examples for different mediums have been performed using the FreeFEM++ software. Switch surfaces for each of them have been predicted using the trained neural network. Mediums can be interpreted as glass, iron, stainless steel, and titanium. The comparison of numerical solutions and neural network predictions is shown in fig. 1.

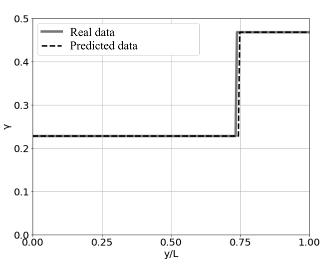
Results specified as “real” in Figure 1 are results of numerical solution of the subdifferential complex heat transfer problem obtained using Newton method in FreeFEM++ software. They are compared to switching points of γ function obtained using the neural network prediction.



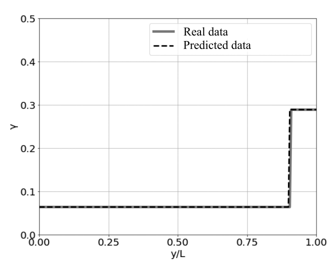
(a) Glass



(b) Iron



(c) Stainless steel



(d) Titanium

Fig. 1: Comparison of real and predicted γ switch points.

3 Conclusion

The deep learning method to solve the subdifferential boundary value problem of complex heat transfer was utilized. To form the dataset, 16,000 forward problems for the complex heat transfer model have been solved numerically using FreeFEM++ software. Deep learning model prediction has shown high accuracy. Examples for different mediums are presented. Thus, deep learning has shown great potential to solve non-standard problems of subdifferential type.

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АННОТАЦИЯ

В работе рассмотрены задачи сложного теплообмена. Предлагается метод для нахождения поверхности переключения, основанный на глубоком обучении. В методе используется обученная на базе данных численных решений прямой задачи нестационарного сложного теплообмена нейронная сеть. Полученные результаты были верифицированы путем сравнения с результатами численных экспериментов.

Ключевые слова: *субдифференциальная краевая задача, глубокое обучение, нейронные сети, сложный теплообмен.*