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MATHEMATICAL MODELING AND MACHINE LEARNING TECHNIQUES IN SOLVING THE HEAT TRANSFER INVERSE PROBLEMS

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Abstract
Using temperature values in 2D-space and its variations in time as well as the boundary conditions for both temperatures and vapor pressure an inverse problem has been studied in attempt to infer the conductivity properties of the domain by using the physics informed neural networks. Relying on mathematical models of heat and moisture transfer a set of criteria has been proposed to form the loss functions to train the networks for temperature, vapor pressure, heat flux and conductivity predictions. The neural networks have been trained by using the proposed loss functions and the conductivity coefficients have been approximated to a certain level of accuracy. The results have shown good correlation of predictions to the ground truth values thus confirming good potential of the method and its ability to solve the problems provided that the sufficient number of training epochs have been used. Simultaneous and coupled training of few networks at a time has shown expectedly slow convergency.

1 General

Ability to solve the inverse problems is an important tool that allows to monitor the performance of the structures by inference from some easy-to-measure indirect data. Machine learning methods and techniques renown as physically informed neural networks (PINN) supported by mathematical modeling frameworks, allowed to incorporate the physics laws into the regression analysis thus increasing the accuracy and soundness of the solutions. Present paper studies an application of PINN technique for solving an inverse problem in heat transfer, namely, it discusses an attempt to predict the ongoing change in the thermal conductivity parameters of the materials composing an exterior wall, by analyzing the variation of temperatures both in space and time within the non-uniform fragment of such a wall. This temperature variation was the result of combined action of different phenomena such as heat transfer, moisture transfer, vapor condensation and evaporation caused by varying in time boundary conditions.

The solution of non-linear, coupled, time-dependent heat transfer problem in two-dimensional space is given in paper [1], that has been used as a source data in the present study. Figure 1 depicts a multi-layered wall and floor slab connection detail, which is used as the model [1].

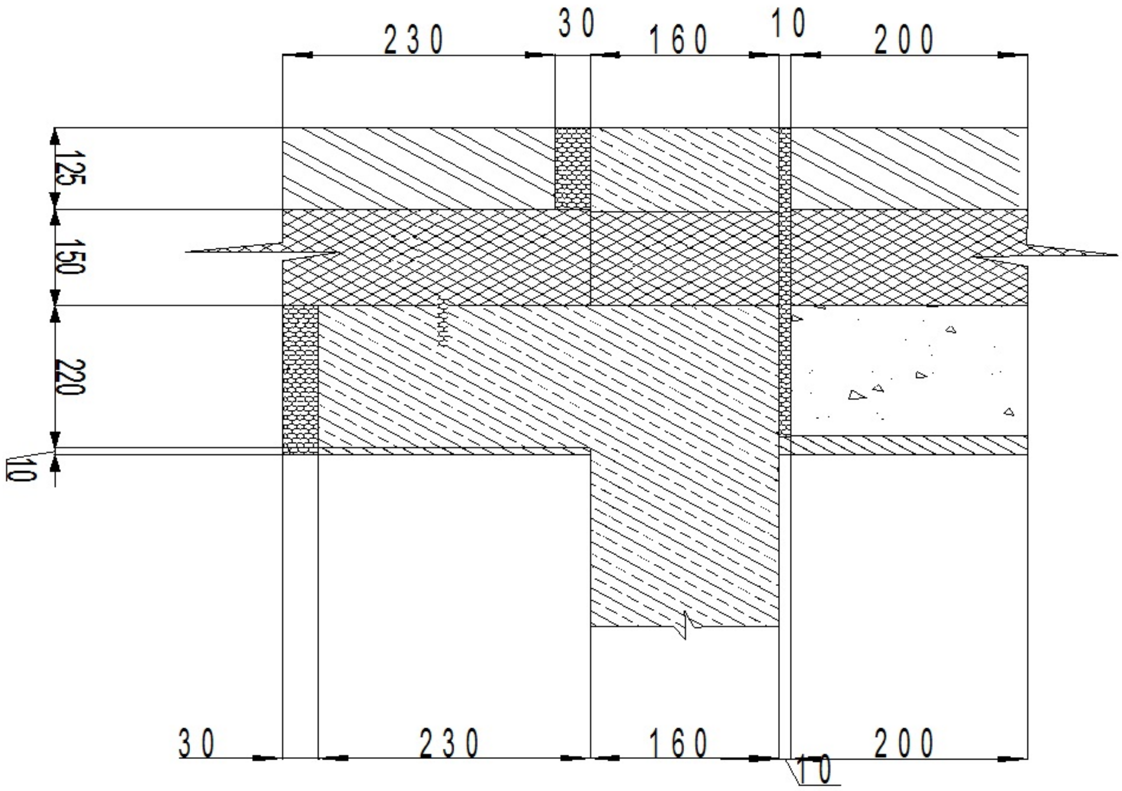

Figure 1 – Connection detail of three-layered exterior wall to concrete floor slab. Source "Energy efficient exterior walls with brick veneer. Details. Wall type 1, detail 1 (to section 2–2)" [2]. All dimensions are in mm

1.1 Given

Let spatial and temporal variables be defined as $x, y, t \in (\Omega \times T)$, where Ω is spatial domain, and T is temporal domain, x, y – spatial coordinates covering the model (Figure 1). Temperature distribution within the model is given in a discrete form [1] and constitutes the input data or the ground truth for the inverse problem. This data can be written as:

$$\Phi: (x, y \in \mathbb{R}^{207\times 2}, t \in \mathbb{R}^{200}) \mapsto \phi \in \mathbb{R}^{207\times 200}, \quad (1)$$

where

$x, y, t \in (\Omega \times T)$;

Φ – an operator that maps spatial and temporal variables to temperature values;

ϕ – temperatures ℃.

Additionally, mixed boundary conditions (Robin conditions) for the temperature (time dependent variation of heat fluxes and the temperature itself) and Dirichlet boundary conditions for the vapor pressure (time dependent variation of relative humidity indoor and outdoor) are also considered as given [1]. All materials are isotropic. It is also known that conductivities are linearly dependent on material moisture content.

1.2 Problem Definition

Having information above, we need to find a function that will correlate the spatial and temporal variables to conductivity coefficient, i. e.

$$\mathcal{D}: (x, y, t) \in \Omega \times T \mapsto \widetilde{D}, \tag{2}$$

where

$\widetilde{D}$ – conductivity coefficient approximation;

$\mathcal{D}$ – function that maps (x, y, t) to conductivity coefficient values.

Heat sinks and sources Q_h are being calculated by using the following expression [1]:

$$Q_h = 595\, \Theta\, A \left(\frac{0.0022\, k_B}{p_{atm}\, m} p - \frac{0.0022\, k_B}{p_{atm}\, m} 610.94\, e^{\left(\frac{17.625\, \phi}{\phi + 243.04}\right)} \right), \tag{3}$$

where

p – vapor pressure within Ω;

ϕ – temperature, °C;

$\Theta = (25 + 19\, v)$ – evaporation coefficient in $\frac{kg}{m^2\, hour}$, v – air flow velocity in $\frac{m}{sec}$, which is set to zero;

A – moisture to air contact area, m^2;

p_{atm} – absolute pressure in Pa (atmospheric pressure);

m – dry air molecular mass;

k_B – Boltzmann constant.

Variation of vapor pressure within Ω is unknown and need to be approximated in form of:

$$\mathcal{P}: (x, y, t) \in \Omega \times T \mapsto \tilde{P}, \tag{4}$$

where

$\tilde{P}$ – approximate values of vapor pressure in (x, y) at any time t;

$\mathcal{P}$ – a function that maps $(x, y, t) \in \Omega \times T$ to vapor pressure values.

2 Materials and Methods

2.1 Neural Networks

Let seek all unknown functions in form of the neural networks, such that:

$$\widetilde{D} = D_{min} + (D_{max} - D_{min})\, \sigma\big(NN_{\mathcal{D}}(x, y, t; \theta_D)\big), \tag{5}$$

where

$\widetilde{D}$ – approximate values of conductivity coefficient;

D_{min}, D_{max} – minimum and maximum possible values of conductivity coefficients within the domain. This is a-priori information aimed to limit the solution of ill-posed problem to a pre-set range. Maximum and minimum values of conductivities for materials that are usual in construction industry are known from the literature [4];

$\sigma(\cdot)$ – sigmoid function with a range [0,1];

$NN_{\mathcal{D}}$ – a neural network;

x, y, t – spatial and temporal arguments defined in $\Omega \times T$;

θ_D – neural network parameters.

Similarly, for (4), the vapor pressure function shall have the form of:

$$\tilde{P} = P_{out}(t) + \left(P_{in}(t) - P_{out}(t)\right)\sigma\left(NN_{\mathcal{P}}(x, y, t; \theta_P)\right), \tag{6}$$

where

$\tilde{P}$ – vapor pressure approximation;

$P_{in}(t), P_{out}(t)$ – vapor pressure values at inner and outer face of the wall at a time t – the boundary conditions;

$NN_{\mathcal{P}}$ – a neural network;

θ_P – neural network parameters;

see (5) for others.

Additionally, we introduce the following functions:

– Normalized temperature as a function of space and time

$$\bar{\phi} = \sigma\left(NN_{\phi}\left(x, y, t; \theta_{\phi}\right)\right), \tag{7}$$

where

$\bar{\phi}$ – approximate values of temperatures normalized to a range of [0,1];

NN_{ϕ} – neural network;

θ_{ϕ} – neural network parameters;

see (5) for others. This function is normalized continuous form of (1).

– Heat flux vector function of space and time

$$\{\widetilde{Jh}\} = Jh_{min} + (Jh_{max} - Jh_{min})\,\sigma\left(NN_J\left(x, y, t; \theta_J\right)\right), \tag{8}$$

where

$\{\widetilde{Jh}\}$ – a vector $\left(\widetilde{Jh}_x, \widetilde{Jh}_y\right)$ of heat flux at x, y, t;

Jh_{min} , Jh_{max} – minimum and maximum possible values of heat flux with in $\Omega \times T$, that can be approximated from Robin boundary conditions for the temperatures;

NN_J – neural network generating a vector $\left\{NN_{Jx}, NN_{Jy}\right\}^T$;

θ_J – neural network parameters;

see (5) for others.

2.2 Loss functions

In order to train the networks, or, in other words, to determine network parameters we need to build, so called, loss functions that will be used in optimization calculations. The following criteria are proposed to evaluate how accurate the predictions are, on one side and to regularize them to avoid the overfitting.

2.2.1 Neural network for prediction of temperatures (7)

a) "Prediction versus the Ground Truth" Criterion – Supervised Learning

$$\mathcal{L}\phi_1 = \|\bar{\phi} - \phi\|_2 , \tag{9}$$

where

$\bar{\phi}$ – temperature predictions by neural network for $(x, y, t) \in \Omega \times T$;

ϕ – temperature values as per (1) for the same $(x, y, t) \in \Omega \times T$, the ground truth;

b) Regularization Criteria

$$\mathcal{L}_{\Phi_2} = ||\overline{\Phi_x}||_2 + ||\overline{\Phi_y}||_2 \quad (10)$$

$$\mathcal{L}_{\Phi_3} = ||\overline{\Phi_{xx}}||_2 + ||\overline{\Phi_{yy}}||_2 \quad (11)$$

$$\mathcal{L}_{\Phi_4} = ||\overline{\Phi_{xxx}}||_2 + ||\overline{\Phi_{yyy}}||_2 \quad (12)$$

where

$\bar{\phi}_x = \frac{\partial \bar{\phi}}{\partial x}$ – first partial derivative of temperature predictions over x;

$\bar{\phi}_y = \frac{\partial \bar{\phi}}{\partial y}$ – first partial derivative of temperature predictions over y;

$\bar{\phi}_{xx} = \frac{\partial^2 \bar{\phi}}{\partial x^2}$ – second partial derivative of temperature predictions over x;

$\bar{\phi}_{yy} = \frac{\partial^2 \bar{\phi}}{\partial y^2}$ - second partial derivative of temperature predictions over y;

$\bar{\phi}_{xxx} = \frac{\partial^3 \bar{\phi}}{\partial x^3}$ - third partial derivative of temperature predictions over x;

$\bar{\phi}_{yyy} = \frac{\partial^3 \bar{\phi}}{\partial y^3}$ - third partial derivative of temperature predictions over y;

c) "Predicted Time Derivative versus Ground Truth Time Derivative" Criterion – Supervised Learning

$$\mathcal{L}\Phi_5 = \|\bar{\phi}_t - \phi_t\|_2, \quad (13)$$

where

$\bar{\phi}_t = \frac{\partial \bar{\phi}}{\partial t}$ – first partial derivative of temperature predictions over time;

ϕ_t – first partial derivative of temperature over time as per (1), calculated by using finite differences method.

d) "Fourier's Law" Criteria

As per Fourier's Law [5], the heat flux predictions of (8) can be assessed jointly with temperature predictions (7) and conductivity predictions (5) by the following equations:

$$\mathcal{L}\Phi_6 = \left\| \widetilde{Jh}_x + \widetilde{D} \frac{\partial \bar{\phi}}{\partial x} \right\|_2 \quad (14)$$

$$\mathcal{L}\Phi_7 = \left\| \widetilde{Jh}_y + \widetilde{D} \frac{\partial \bar{\phi}}{\partial y} \right\|_2 \quad , \quad (15)$$

where

$\widetilde{Jh}_x$ – heat flux at x direction as predicted by (8);

$\widetilde{Jh}_y$ – heat flux at y direction as predicted by (8);

$\widetilde{D}$ – conductivity coefficients as predicted by (5);

$\frac{\partial \bar{\phi}}{\partial x}, \frac{\partial \bar{\phi}}{\partial y}$ – spatial derivatives of temperature predictions $\bar{\phi}$ at x, y directions respectively;

e) "Heat Balance Equation" Criterion

$$\mathcal{L}\Phi_8 = \left\| -\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial}{\partial x}\left(\widetilde{D} \frac{\partial \bar{\phi}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\widetilde{D} \frac{\partial \bar{\phi}}{\partial y}\right) + Q_h\left(\tilde{P}, \bar{\phi}\right) \right\|_2, \quad (16)$$

where

$Q_h\left(\tilde{P}, \bar{\phi}\right)$ – an energy consumed/expelled during evaporation/condensation as per (3)

$$Q_h(\tilde{P},\bar{\phi}) = 595\,\Theta\,A\left(\frac{0.0022\,k_B}{p_{atm}\,m}\tilde{P} - \frac{0.0022\,k_B}{p_{atm}\,m}610.94\,e^{\left(\frac{17.625\,\bar{\phi}}{\bar{\phi}+243.04}\right)}\right), \quad (17)$$

$\frac{\partial\bar{\phi}}{\partial t}$ – temporal derivative of temperature predictions $\bar{\phi}$;

others see (14), (15);

f) "Gauss – Green Theorem" Criterion.

Gauss – Green theorem correlates the changes of a vector field within a closed area to the changes of that field along the boundary of the same area.

$$\mathcal{L}\phi_9 = \|J_{bc}^{\omega} + J_{in}^{\omega}\|_2, \quad (18)$$

where

$$J_{bc}^{\omega} \;=\; \oint_S \left(\widetilde{D}\frac{\partial\bar{\phi}}{\partial x}cos(\alpha) + \widetilde{D}\frac{\partial\bar{\phi}}{\partial y}sin(\alpha)\right)dS; \quad (19)$$

$$J_{in}^{\omega} \;=\; \iint_{\omega}\left(\frac{\partial}{\partial x}\left(\widetilde{D}\frac{\partial\bar{\phi}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\widetilde{D}\frac{\partial\bar{\phi}}{\partial y}\right) + Q_h(\tilde{P},\bar{\phi})\right)d\omega, \quad (20)$$

where

α – an angle between positive x direction and an outward normal to boundary S of subdomain ω such that;

$\Omega = \bigcup_{i=1}^{N}\omega_i$, where N – number of subdomains;

J_{bc}^{ω} – total heat flux change along the boundary of the subdomain ω;

J_{in}^{ω} – total heat flux change within ω.

Having specified the criteria above, the total loss function for this network then might be presented as their sum.

$$\mathcal{L}\phi = \sum_{i=1}^{9}\mathcal{L}\phi_i. \quad (21)$$

In order to determine the parameters of the neural networks the following optimization problem needs to be solved.

$$\theta_{\phi} = argmin_{\theta_{\phi}}(\mathcal{L}\phi) = \{(x,y,t) \in \Omega \times T : \mathcal{L}\phi(x,y,t) \le \epsilon\}, \quad (22)$$

where ϵ – accuracy of the solution.

2.2.2 Neural Network for Prediction of Vapor Pressure (6)

Let denote as $p_{bc} = \{p_{in}, p_{out}\}^T$ the vapor pressures values at the boundaries of Ω, being given as Dirichlet boundary conditions as per [1]. Also, let $\partial\Omega_{in}$ be a boundary of Ω facing the indoor environment and $\partial\Omega_{out}$ – a boundary facing the outdoor environment, then:

a) "Prediction versus Boundary Conditions" Criteria

$$\mathcal{L}\wp_1 = \left\|\tilde{P}(\partial\Omega_{in} \vee \partial\Omega_{out}) - p_{bc}\right\|_2; \quad (23)$$

b) "Phase Change Heat" Criterion

$$\mathcal{L}\wp_2 = \left\|Q_h^{(1)}(\tilde{P},\bar{\phi}) - Q_h^{(2)}(\tilde{P},\bar{\phi})\right\|_2, \quad (24)$$

where

$$Q_h^{(1)}(\tilde{P},\bar{\phi}) = \frac{\partial\bar{\phi}}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial\bar{\phi}}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial\bar{\phi}}{\partial y}\right); \quad (25)$$

$$Q_h^{(2)}(\tilde{P},\bar{\phi}) = 595\,\Theta\,A\left(\frac{0.0022\,k_B}{p_{atm}\,m}\tilde{P} - \frac{0.0022\,k_B}{p_{atm}\,m}610.94\,e^{\left(\frac{17.625\,\bar{\phi}}{\bar{\phi}+243.04}\right)}\right), \quad (26)$$

$\widetilde{D}$ – conductivity coefficients as predicted by (5);

c) "First Derivatives" as Regularization

$$\mathcal{L}_{\mathcal{P}_3} = \|\tilde{P}_x\|_2 + \|\tilde{P}_y\|_2 + \|\tilde{P}_t\|_2, \quad (27)$$

where

$\tilde{P}_x = \frac{\partial \tilde{P}}{\partial x}$ – first partial derivative of vapor pressure over x;

$\tilde{P}_y = \frac{\partial \tilde{P}}{\partial y}$ - first partial derivative of vapor pressure over y;

$\tilde{P}_t = \frac{\partial \tilde{P}}{\partial t}$ – first partial derivative of vapor pressure over time;

d) "Prediction to be Close to Mean" Criterion.

As a regularization criterion it is assumed that the predicted vapor pressure values need to be close to mean values calculated as a linear interpolation across the domain Ω, between its boundary values.

$$\mathcal{L}_{\mathcal{P}_4} = \|\tilde{P} - \hat{P}\|_2, \quad (28)$$

where

$$\hat{P} = p_{out} + \frac{p_{in} - p_{out}}{\Omega}(x, y, t), \quad (29)$$

$\hat{P}$ – linear interpolation between p_{in}, p_{out} within Ω at any given time t;

$(x, y, t) \in \Omega \times T$.

Total loss function for this network will have a form of:

$$\mathcal{L}_{\mathcal{P}} = \sum_{i=1}^{4} \mathcal{L}_{\mathcal{P}_i}. \quad (30)$$

Optimization problem to determine network parameters has the following form:

$$\theta_p = argmin_{\theta_p}(\mathcal{L}_{\mathcal{P}}) = \{(x, y, t) \in \Omega \times T : \mathcal{L}_{\mathcal{P}}(x, y, t) \le \epsilon\} \quad (31)$$

where ϵ – accuracy of the solution.

2.2.3 Neural Network for Prediction of Heat Flux Values (8)

The following criteria shall be used for training of heat flux neural network.

a) "Predictions versus Robin Boundary Conditions" Criterion

$$\mathcal{L}_{\mathcal{J}_1} = \left\| \sqrt{(\tilde{J}h_{in})_x^2 + (\widetilde{Jh_{in}})_y^2} - Jh_{in} \right\|_2 + \left\| \sqrt{(\tilde{J}h_{out})_x^2 + (\widetilde{Jh_{out}})_y^2} - Jh_{out} \right\|_2, \quad (32)$$

where

Jh_{in}, Jh_{out} – heat flux values at inner and outer face of Ω at a time t – Robin boundary conditions;

$(\tilde{J}h_{in\,x}, \tilde{J}h_{in\,y})$ – neural network prediction for heat flux at $\partial\Omega_{in}$;

$(\tilde{J}h_{out\,x}, \tilde{J}h_{out\,y})$ – neural network prediction for heat flux at $\partial\Omega_{out}$;

b) "Prediction to be Close to Mean" as Regularization Criterion.

$$L_{J_2} = \||\tilde{J}h_{tot}(x, t) - \hat{J}h(x, t)|\|_2, \quad (33)$$

where

$\tilde{J}h_{tot}(x, t)$ – heat flux as predicted by neural network (8), passing through a plane along y direction and at any given x and time t.

$$\tilde{J}h_{tot}(x, t) = \int_{y_{min}}^{y_{max}} \tilde{J}h\,(x, t)dy. \quad (34)$$

$\hat{J}h(x, t)$ – heat flux passing through a vertical plane at any given x, in a moment t, being calculated as linear interpolation between boundary values;

$$Jt_{out}(t) = \int_{\Omega_{out}} J\,h_{out}(t)\,d\Omega_{out}\,; \tag{35}$$

$$Jt_{in}(t) = \int_{\Omega_{in}} J\,h_{out}(t)\,d\Omega_{in}\,; \tag{36}$$

$$\widehat{Jh}(x,t) = Jt_{out} + \frac{Jt_{in} - Jt_{out}}{\Omega}(x,t)\,; \tag{37}$$

$Jt_{out}(t), Jt_{in}(t)$ – total heat flux leaving and entering Ω at time t, respectively;
(x,t) – x coordinate and time argument t;
c) "Heat Flux Direction" Criterion.

From Fourier's Law we know that heat flux needs to be opposite directed to the space derivatives of the temperature. Hence

$$\mathcal{L}_{\mathcal{J}_3} = ||\overline{\varphi}_x^{\text{norm}} + \tilde{J}h_x^{\text{norm}}||_2 + ||\overline{\varphi}_y^{\text{norm}} + \tilde{J}h_y^{\text{norm}}||_2\,, \tag{38}$$

where

$\nabla\bar{\phi}^{norm} = \left(\bar{\phi}_x^{norm}, \bar{\phi}_y^{norm}\right)$ – unit vector of temperature gradients, predicted by neural network (7);

$\widetilde{Jh}^{norm} = \left(\widetilde{Jh}_x^{norm}, \widetilde{Jh}_y^{norm}\right)$ – unit vector of heat flux, predicted by neural network (8);

d) "Heat Balance Equation" Criterion

$$\mathcal{L}_{\mathcal{J}_4} = ||-\frac{\partial\bar{\Phi}}{\partial t} + \frac{\partial\widetilde{\text{Jh}}_\text{x}}{\partial x} + \frac{\partial\widetilde{\text{Jh}}_\text{y}}{\partial y} + Q_h(\bar{P},\bar{\Phi})\,||_2\,; \tag{39}$$

$\frac{\partial\widetilde{\text{Jh}}_\text{x}}{\partial x}, \frac{\partial\widetilde{\text{Jh}}_\text{y}}{\partial y}$ – space derivatives of heat flux predictions;

e) "Gauss – Green Theorem" Criterion

$$\mathcal{L}_{\mathcal{J}_5} = \|J_{bc}^{\omega} + J_{in}^{\omega}\|_2\,, \tag{40}$$

where

$$J_{bc}^{\omega} = \oint_S \left(\widetilde{J}h_x + \widetilde{J}h_y\right) dS, \tag{41}$$

$$J_{in}^{\omega} = \iint_{\omega} \left(\frac{\partial\widetilde{J}h_x}{\partial x} + \frac{\partial\widetilde{J}h_y}{\partial y} + Q_h\left(\tilde{P},\bar{\phi}\right)\right) d\omega\,. \tag{42}$$

Total loss function for neural network (8) is then:

$$\mathcal{L}_{\mathcal{J}} = \textstyle\sum_{i=1}^{5} \mathcal{L}_{\mathcal{J}_i}\,. \tag{43}$$

In order to determine the network parameters, the following optimization problem need to be solved:

$$\theta_J = argmin_{\theta_J}\left(\mathcal{L}_{\mathcal{J}}\right) = \left\{(x,y,t) \in \Omega \times T : \mathcal{L}_{\mathcal{J}}(x,y,t) \le \epsilon\right\}, \tag{44}$$

where ϵ – accuracy of the solution.

2.2.4 Neural Network for Prediction of Conductivity Coefficients (5)

The criteria for this network are:

a) "Heat Balance Equation" Criterion

$$\mathcal{L}_{\mathcal{D}_1} = \left\|-\frac{\partial\bar{\phi}}{\partial t} + \frac{\partial}{\partial x}\left(\widetilde{D}\frac{\partial\bar{\phi}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\widetilde{D}\frac{\partial\bar{\phi}}{\partial y}\right) + Q_h\left(\tilde{P},\bar{\phi}\right)\right\|_2; \tag{45}$$

b) "Fourier's Law" Criteria

$$\mathcal{L}_{\mathcal{D}_2} = ||\tilde{J}h_x + \widetilde{D}\frac{\partial\bar{\Phi}}{\partial x}||_2 \, ; \tag{46}$$

$$\mathcal{L}_{\mathcal{D}_3} = ||\tilde{J}h_y + \widetilde{D}\frac{\partial\bar{\Phi}}{\partial y}||_2 \, ; \tag{47}$$

c) "Gauss – Green Theorem" Criterion

$$\mathcal{L}_{D4} = ||J_{bc}^{\omega} + J_{in}^{\omega}||_2 \, , \tag{48}$$

where

$J_{bc}^{\omega}, J_{in}^{\omega}$ – the same as in (19) and (20).

Total loss function is then:

$$\mathcal{L}_{\mathcal{D}} = \sum_{i=1}^{4} \mathcal{L}_{\mathcal{D}i} \, . \tag{49}$$

Similar to other networks the optimization problem to find network parameters has a form:

$$\theta_D = argmin_{\theta_D}(\mathcal{L}_{\mathcal{D}}) = \{(x, y, t) \in \Omega \times T : \mathcal{L}_{\mathcal{D}}(x, y, t) \leq \epsilon\}, \tag{50}$$

where ϵ – accuracy of the solution.

2.3 Training

While the training of the networks the relevant loss functions were weighted by adaptive Lagrange multipliers as recommended in [7].

$$\mathcal{L}_{\mathcal{NN}} = \sum_{i=1}^{N}\left(\lambda_i \mathcal{L}_i + \frac{1}{2}\log\left(\frac{1}{2\lambda_i}\right)\right), \tag{51}$$

where

$\mathcal{L}_{NN}$ – total loss function of N^{th} (or respective) neural network;

N – number of criteria of relevant loss function;

λ_i – Lagrange coefficient, such that

$$\lambda_i = \frac{1}{2\left(s_{(i)}^2 + \gamma^{-1}\right)}, \tag{52}$$

where

i – index of associated criterion;

γ^{-1} – top limit for Lagrange coefficients [7];

$s_{(i)}^2$ – variance of residuals for i^{th} criterion of associated loss function. For instance, for 4th criterion of network (8) the variance is calculated as:

$$s_{(4)}^2 = \frac{\sum_{j=1}^{N}\left((J_{bc}^{\omega})_j - (-J_{in}^{\omega})_j\right)^2}{N-1}, \tag{53}$$

N – number of values in a training batch.

3 Results

Neural networks architecture and training parameters are given in Table 1.

Figure 2 shows (a) the temperature distribution within the domain as it is predicted by neural network (7) upon completion of first stage of training and (b) the ground truth values as per (1). First stage training was performed by using supervised learning criteria only. Relative error is amounted up to 30 %. Second training stage was coupled as all four networks were trained simultaneously by using each other's predictions in their respective loss functions. Figure 3 depicts the ground truth temperatures as per (1) and neural network (7) predictions after the second stage of training.

Table 1 – Neural Networks' Architectures

Item	Neural Network for Temperatures (7)	Neural Network for Heat flux (8)	Neural Network for Vapor Pressure (6)	Neural Network for Conductivity Coefficient (5)
Input layer. Number of neurons (x, y, t)	3	3	3	3
Number of output neurons	1	2	1	1
Number of hidden layers	7	6	5	5
Number of neurons in hidden layers				
Hidden Layer 1	40	15	20	20
Hidden Layer 2	25	20	20	20
Hidden Layer 3	30	30	20	20
Hidden Layer 4	40	25	20	20
Hidden Layer 5	30	20	20	20
Hidden Layer 6	25	15	–	–
Hidden Layer 7	40	–	–	–
Skip connections	1 → 7, 2 → 6	1 → 6, 2 → 5	1 → 5, 2 → 4	1 → 5, 2 → 4
Training curriculum	2 staged	Single staged	Single staged	Single staged
Number of epochs	40000+10000	10000	10000	10000

a) b)

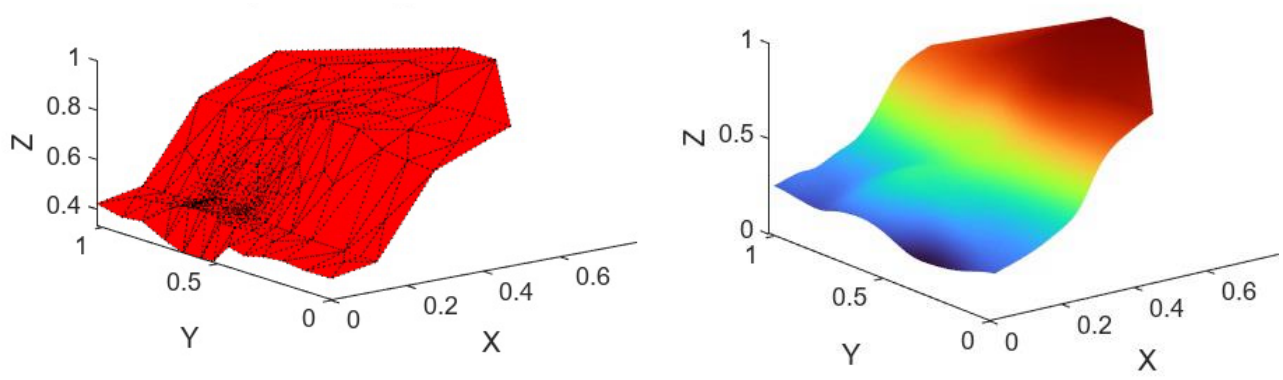

Figure 2 – The temperature values (a) the ground truth values as per (1); (b) predictions of the neural network (7) after first stage of training. X, Y – spatial coordinates in Ω, Z – normalized temperature values. The values are given for a moment of t = 0.32663

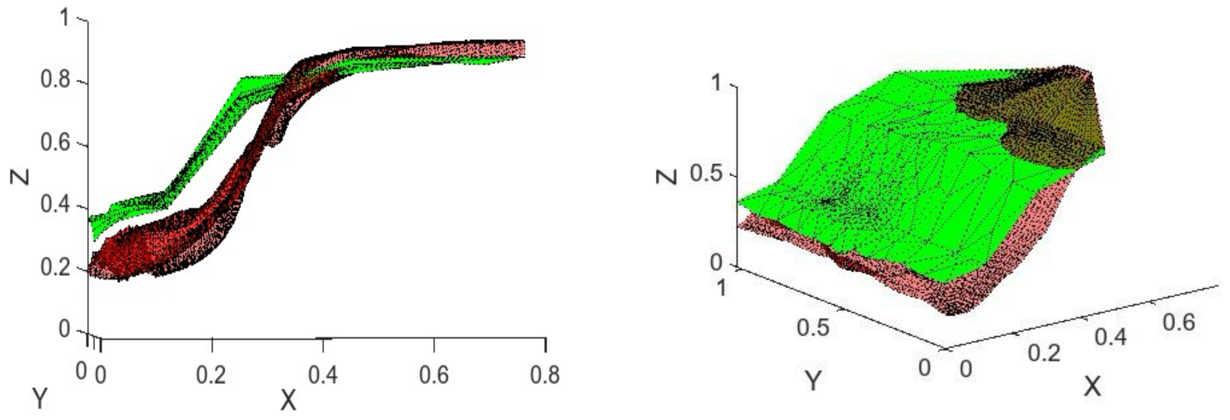

Figure 3 – The temperature values at time $t = 0.94472$. Green – ground truth (1), red – prediction of (7). X, Y – spatial coordinates in Ω, Z – normalized temperature values

Relative error has increased till 40 % due to inclusion of other networks into training process that has negatively affected the predictions temperature network (7).

Figure 4 shows vapor pressure values predicted by neural network (6) in comparison with values obtained in [1]. As it was noted above, the training of this network has been carried out by using the boundary conditions and indirect criteria (24) and (25).

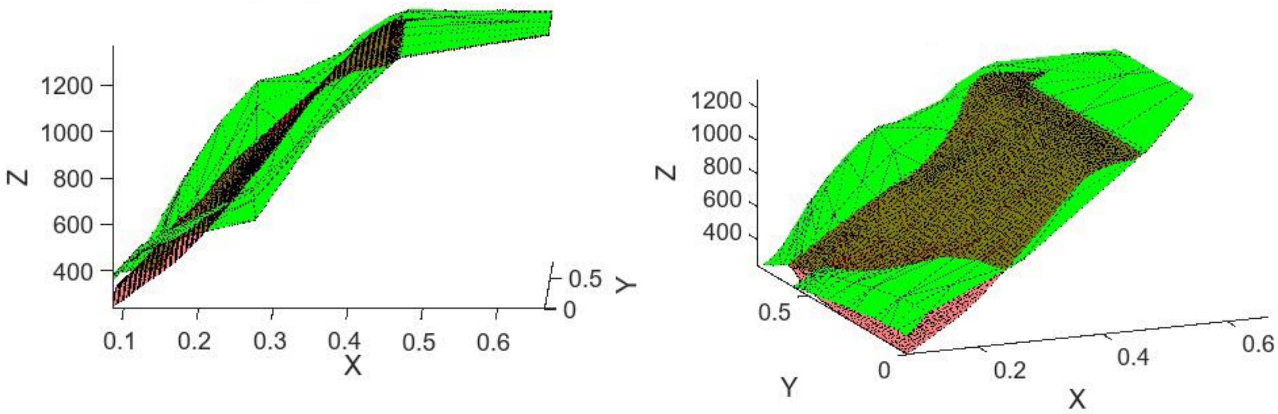

Figure 4 – Vapor pressure values within Ω at time $t = 0.94472$. Green – ground truth values [1], red – predictions of (6). X, Y – spatial coordinates in Ω, Z – vapor pressure values

Figure 5 shows the values of conductivity coefficients as predicted by neural network (5) in comparison to data in [1]. The highest error values are occurring in this network's predictions as they aggregate the errors of all other networks.

Figure 6 depicts Forbenius norms for space and time series of conductivity coefficient predictions over $(\Omega \times T)$. As it can be seen, the proposed loss functions indeed train the networks, however more epochs and further refinements are needed to reduce the training errors.

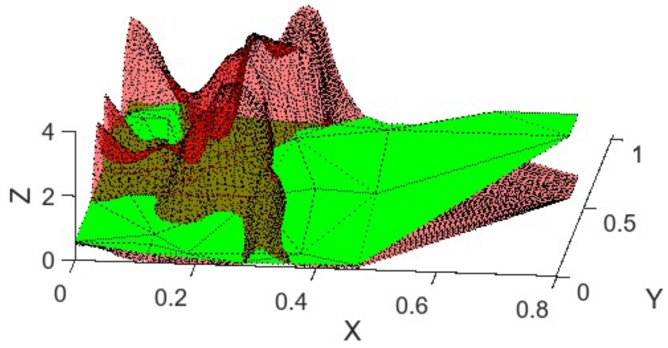

Figure 5 – Conductivity coefficients at time t = 0.94472. Green – ground truth values [1], red – predictions of neural network (5). X, Y – spatial coordinates in Ω, Z – conductivity coefficient values

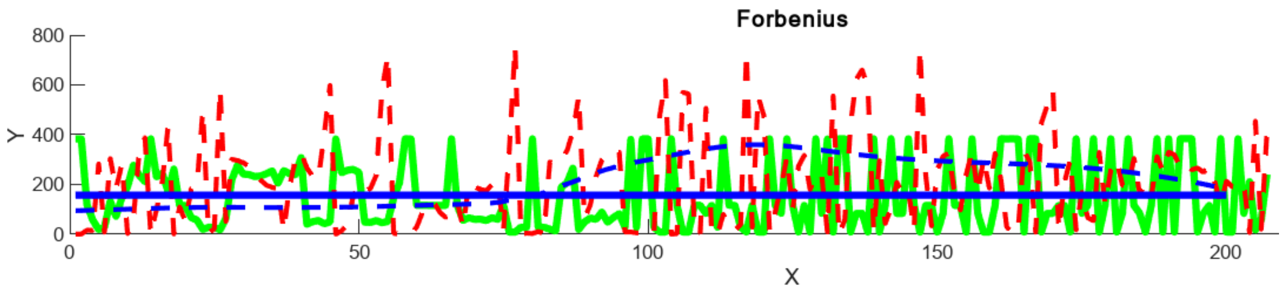

Figure 6 – Forbenius norms. Green solid line (Y) – Forbenius norm values of all spatial collocation points $(x, y) \in \Omega$ as per the ground truth data (1); Red dashed line (Y) – Forbenius norm values of all spatial collocation points $(x, y) \in \Omega$ as predicted by neural network (5), (X) time steps $t \in T$; Blue solid line (Y) – Forbenius norm through all time steps of each collocation point $(x, y) \in \Omega$ of ground truth values; Blue dashed line (Y) – Forbenius norm through all time steps of each collocation point $(x, y) \in \Omega$ as predicted by (5), (X) collocation point number

4 Conclusions

At the result of the study, the followings might be concluded:

1. Inverse problems are knowingly ill-posed, therefore every problem requires an individual strategy for its solving. In case of neural network, due care needs to be given to proper selection of loss function criteria.

2. Mathematical models of heat and moisture transfer and the underlying physics laws adopted in training criteria allow to train the networks even with limited ground truth data.

3. Having properly selected the training criteria, the machine learning techniques become powerful and effective tools for solving the inverse problems. As equally, the architecture of the networks should be carefully selected by analyzing the particularities of the problem. In the present study, the inclusion of skip connections in network architecture allowed to avoid gradient vanishing problem.

4. Large number of criteria combined in a loss function may complicate the training process, therefore a contribution of each criterion needs to be adjusted dynamically during the training. Adaptive Lagrange coefficients allow to level or magnify the effect of any single criterion thus to dose them as relevant during the training process.

5. Coupled inverse problems require prolonged training time as the optimization needs to be achieved in all neural networks simultaneously.

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