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Investigation of the Performance of Machine Learning Algorithms of Casson-Micropolar Nano Particles Around a Cylindrical Shape: ANN and PINN

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Abstract

Present study deals with a comprehensive analysis of Micropolar-Casson fluid model in two dimensional through a porous cylinder. In order to represent an accurate complex transport scenario encountered in Industrial and engineering applications formulated mathematical model incorporates Joule heating, heat source, mixed convection, chemical reaction and radiation. Convective boundary conditions were assumed. Non-similar transformations were employed to proposed system of nonlinear equations to get ordinary equations. Transformed system of nonlinear differential equations were resolved via two intelligence-based approaches i.e. Physics-informed neural network and artificial neural network. PINN based predictivity is examined at different number of iterations i.e. 1000-20,000. Mean absolute error decays as we increased number of epochs. ANN and PINN based highly authentic and stable solutions compared with BVP4c solutions were obtained. Comprehensive analysis of ANN\PINN and BVp4c shows overlapped, stable, authentic and convergent outcomes at 20,000 epochs. It guarantees efficient, robustness and reliable approach for solving nonlinear system of equations alternate to conventional numerical approaches.

Keywords: Physics-informed neural network; Porous media; Thermal radiation, Joule heating; mixed convection.

1. Introduction

The non-Newtonian fluids have been of great interest to many scientists because of the variety of uses for them. Non-Newtonian fluids are fluids that change resistance to flow under different forces. There are numerous uses for Casson fluid, some of which we address below. Numerous mechanical engineering and biological flow behaviors, such as chocolate, blood, and printing areas, can be utilized. When the force is applied to the particles of the Casson fluid, it flows smoothly, but without applied force, it behaves like a solid. During the motion of fluids, tiny particles can rotate locally, leading to the formation of micropolar fluids. Micropolar has many

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complex engineering applications like this, helping to study flow patterns and heat transfer, making the model authentic. A comparative analysis using HAM and collocation procedures of Casson nanofluid from a vertical convective surface studied by Muhammad Nasir et al. [1]. Majid Hussain et al. [2] explored the work on numerical investigation of Casson fluid through a stretched permeable wedge. Dual solutions of Casson tetra hybrid nanofluid flow in a porous curved surface and stability analysis presented by Tezera Gizewu et al. [3]. Abdullah et al. [4] examined the numerical study of Casson MHD nanofluid flow on an inclined surface. Hassan Waqas et al. [5] examined the computational study of rotational micropolar nanomaterials with activation energy by numerical methods. Numerical investigation of MHD micropolar nanofluid flow configured by the stimulus energies analyzed by M. Ajithkumar et al. [6]. Numerical analysis of micropolar fluid with stagnation point flow via a stretchable sheet extended by Muhammad Salman Kausar et al. [7].

The field of fluid mechanics has many applications wherein the porous media are used to enhance the efficiency of the thermal insulation, fluid flow, and other practical aspects of engineering. A porous medium is a solid type of material that contains tiny, interconnected pores through which a fluid can pass. The modified Darcy-Forchheimer model helps to describe more precisely the behavior of fluid flow via a porous medium than the Darcy scheme, especially for average or high fluid velocities. There are many applications of this model, but relevant to fluid mechanics are well-established uses in biochemical engineering, thermal energy storage systems, heat exchangers, etc. Numerical solutions of hydromagnetic micropolar fluid flow over a stretching sheet in a porous medium investigated by Mayzul A. Hussain et al. [8]. Hamzeh Taha Alkasasbeh et al. [9] flow past an exponentially shrinking surface in a porous medium with the help of MHD Newtonian hybrid nanofluids. Hiranmoy Mait et al. [10] delivered the idea of numerical analysis of nanofluid flow by a stretchable rotating disk in a porous medium. Numerical study of Maxwell fluid in contact with a porous rotating disc explored by Muhammad Faizan et al. [11]. Bhaskar Jyoti Dutta et al. [12] suggested the numerical investigation of MHD mixed convection through a porous medium past a permeable vertical plate. Impacts of a porous medium on the plume generated due to the aligned magnetic field effects are examined by Sahar Anwar et al. [13].

Machine learning plays a vital role in predicting the behavior of fluid flow and heat transfer with high accuracy in fluid mechanics. Machine learning has many techniques but here we discuss two most common and famous for handling the boundary value problems like artificial neural network ANN and physics informed neural network PINN. An artificial neural network, which is a computational model based on the process by which the human brain analyses information. ANN are used to provide fast approximations of numerical data, to talk about the flow of fluid, heat and mass transfer with short interval of time without any repetitive process. The artificial neural network which takes into consideration both observations and physics behind the system is referred to as the Physics Informed Neural Network PINN. PINNs are often employed to predict temperature and velocity fields, as well as to resolve complex partial differential equations. Numerical analysis of ternary hybrid non-Newtonian nanofluid through an inclined shrinking sheet by using ANN studied by Syed Zahir Hussain Shah et al. [14]. Mumtaz Khan et al. [15] presented the numerical study of dynamics in chemically reactive fluids across variable thickness surfaces by using ANN. Study of MHD-based nanofluids past a stretching sheet with the help of ANN with bvp5c explored by Syed Asif Ali Shah et al. [16]. Ikram Ul Haq et al. [17] presented the idea of numerical investigation of MHD micropolar nanofluid with Levenberg–Marquardt algorithm. Using an ANN

to analyze the rheological material and entropy generation are examined by Aneeta Razaq et al. [18]. Shravan Kumar Rudrabhatla et al. [19] studied the numerical investigation of Casson fluid flow by using PINN with viscous dissipation. Reza Nopour et al. [20] performed the numerical analysis of functionally graded reinforced sandwich beams using PINN.

1.1 Novelty

The novelty of the given work is mentioned below in point form:

- ❖ The combination of dual materials like Casson and micropolar nanofluids is used for a vertical cylinder along with the given mathematical model.
- ❖ The combination of effects like mixed convection, Joule heating, thermal radiation, heat source/sink, and chemical reaction along with four profiles like momentum, microrotation, energy, and concentration equations.
- ❖ We applied two powerful techniques to compare the results of ANN and PINN using numerical values, which is a novel aspect of my research work.
- ❖ The connective boundary conditions are helpful to my work, unique compared to the literature review for the same given model with given geometry.
- ❖ Overall, the same work is not available on Google Scholar, and we can say that the given work has a highly novel approach compared to the literature.

2. Mathematical modeling

Here we supposed incompressible, steady and radiated flow via a porous cylinder. While studying Micropolar-Casson fluid flow behavior some effects cannot be ignored i.e. radiation, joule heating, porosity, mixed convection, heat source and chemical reaction. Convective boundary constraints are also taken into consideration. Assumption of these effects increases applicability of model to various industrial and engineering processes involving non-Newtonian fluids. Problem sketch and coordinate system of problem are presented schematically via **Fig. 1**.

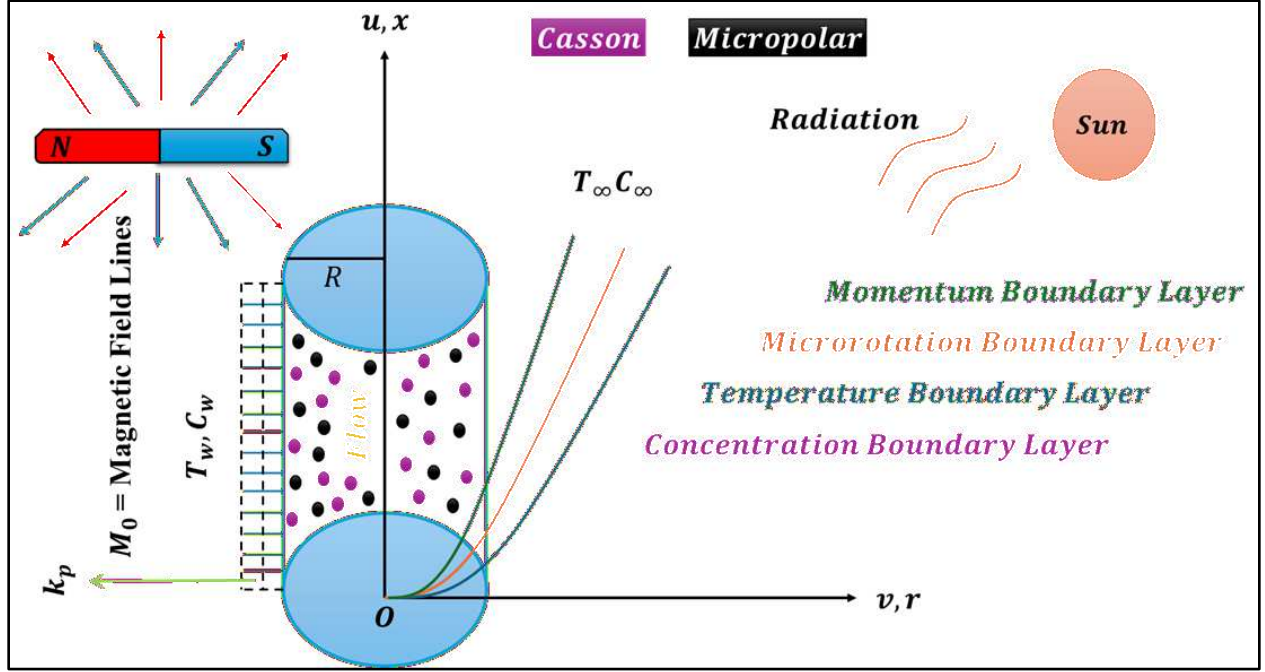


Fig. 1: Problem Sketch.

$$\frac{\partial(rv)}{\partial r} + \frac{\partial(ru)}{\partial x} = 0, \quad (1)$$

$$v \frac{\partial u}{\partial r} + u \frac{\partial u}{\partial x} = \nu_f \left(1 + \frac{1}{C_p} + \frac{k}{\mu_f} \right) \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \right) + \frac{k}{\mu_f} \frac{\partial N}{\partial r} - \frac{\sigma_f B_o^2}{\rho_f} u \quad (2)$$

$$- \left(1 + \frac{1}{C_p} + \frac{k}{\mu_f} \right) \frac{\mu_f}{k_p \rho_f} u + g \{ B_t (T - T_\infty) + B_c (C - C_\infty) \}, \quad (3)$$

$$v \frac{\partial N}{\partial r} + u \frac{\partial N}{\partial x} = \left(\frac{\gamma}{\rho_f J} \right) \left(\frac{\partial^2 N}{\partial r^2} + \frac{1}{r} \frac{\partial N}{\partial r} \right) - \frac{k}{\rho_f J} \left(2N + \frac{\partial u}{\partial r} \right),$$

$$\left[u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial r} \right] = \frac{k_f}{(\rho c_p)_f} \left(\frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} \right) \left(1 + \frac{16\sigma^* T_\infty^3}{3k^* k_f} \right) - \left(1 + \frac{1}{C_p} + \frac{k}{\mu_f} \right) \frac{\mu_f}{k_p (\rho c_p)_f} u^2 \quad (4)$$

$$+ \frac{\sigma_f B_o^2}{(\rho c_p)_f} u^2 + \frac{Q_o}{(\rho c_p)_f} (T - T_\infty),$$

$$\left[v \frac{\partial C^*}{\partial r} + u \frac{\partial C^*}{\partial x} \right] = \left(\frac{\partial^2 C^*}{\partial r^2} + \frac{1}{r} \frac{\partial C^*}{\partial r} \right) D_B - k_r (C^* - C_\infty^*), \quad (5)$$

Boundary conditions

$$\left. \begin{aligned} u = u_w(x), v = 0, N + n \frac{\partial u}{\partial r} = 0, -k_f \frac{\partial T}{\partial r} = h_f(T_w - T), -D_B \frac{\partial C^*}{\partial r} = -h_w(C_w^* - C^*) \text{ at } r = R \\ u \rightarrow 0, N \rightarrow 0, T \rightarrow T_\infty, C^* \rightarrow C_\infty^* \text{ as } r \rightarrow \infty \end{aligned} \right\}, \quad (6)$$

Similarity transformations [21]

$$\left. \begin{aligned} u = u_o \xi \frac{\partial f(\xi, \eta)}{\partial \eta}, v = -\frac{r}{R} \sqrt{\nu_f \frac{u_o}{l}} \left(f(\xi, \eta) + \xi \frac{\partial f(\xi, \eta)}{\partial \xi} \right), \theta(\xi, \eta) = \frac{T - T_\infty}{T_w - T_\infty} \\ \phi(\xi, \eta) = \frac{C^* - C_\infty^*}{C_w^* - C_\infty^*}, \xi = \frac{x}{l}, N = u_o \xi \sqrt{\frac{u_o}{l \nu_f}} g(\xi, \eta), \eta = \frac{r^2 - R^2}{2R} \sqrt{\frac{u_o}{l \nu_f}} \end{aligned} \right\}, \quad (7)$$

We obtain

$$\left(1 + \frac{1}{C_p} + K \right) \left[(1 + 2C\eta) \frac{\partial^3 f}{\partial \eta^3} + 2C \frac{\partial^2 f}{\partial \eta^2} \right] + f \frac{\partial^2 f}{\partial \eta^2} - \left(\frac{\partial f}{\partial \eta} \right)^2 - M \frac{\partial f}{\partial \eta} - K \sqrt{1 + 2C\eta} \frac{\partial g}{\partial \eta} \\ + \frac{L}{\xi} (\theta + N\phi) - \left(1 + \frac{1}{C_p} + K \right) P_m \frac{\partial f}{\partial \eta} = -\xi \left[\frac{\partial^2 f}{\partial \eta^2} \frac{\partial f}{\partial \xi} - \left(\frac{\partial f}{\partial \eta} \right) \frac{\partial^2 f}{\partial \xi \partial \eta} \right], \quad (8)$$

$$S_g \left[(1 + 2C\eta) \frac{\partial^2 g}{\partial \eta^2} + 2C \frac{\partial g}{\partial \eta} \right] + (1 + 2C\eta) f \frac{\partial g}{\partial \eta} - g \frac{\partial f}{\partial \eta} - \left(\frac{\partial f}{\partial \eta} \right)^2 \\ - M_p D_p \left(2g + \sqrt{1 + 2C\eta} \frac{\partial^2 f}{\partial \eta^2} \right) = \xi \left[\frac{\partial f}{\partial \eta} \frac{\partial g}{\partial \xi} - (1 + 2C\eta) \left(\frac{\partial g}{\partial \eta} \right) \frac{\partial f}{\partial \xi} \right], \quad (9)$$

$$\left(1 + \frac{4}{3} R \right) \frac{1}{\text{Pr}} \left[(1 + 2C\eta) \frac{\partial^2 \theta}{\partial \eta^2} + 2C \frac{\partial \theta}{\partial \eta} \right] + f \frac{\partial \theta}{\partial \eta} + MEc \xi^2 \left(\frac{\partial f}{\partial \eta} \right)^2 + Q\theta \\ - \left(1 + \frac{1}{C_p} + K \right) \lambda Ec \xi^2 \left(\frac{\partial f}{\partial \eta} \right)^2 = \xi \left[\frac{\partial \theta}{\partial \xi} \frac{\partial f}{\partial \eta} - \frac{\partial \theta}{\partial \eta} \frac{\partial f}{\partial \xi} \right], \quad (10)$$

$$\frac{1}{Sc} \left[(1 + 2C\eta) \frac{\partial^2 \phi}{\partial \eta^2} + 2C \frac{\partial \phi}{\partial \eta} \right] + f \frac{\partial \phi}{\partial \eta} - Cr\phi = \xi \left[\frac{\partial \phi}{\partial \xi} \frac{\partial f}{\partial \eta} - \frac{\partial \phi}{\partial \eta} \frac{\partial f}{\partial \xi} \right], \quad (11)$$

$$\left. \begin{aligned} \frac{\partial f}{\partial \eta} = 1, f + \frac{\partial f}{\partial \xi} \xi = 0, g + \eta f'' = 0, \frac{\partial \theta}{\partial \eta} = -A(1 - \theta), \frac{\partial \phi}{\partial \eta} = -B(1 - \phi) \text{ (at } \eta = 0) \\ \frac{\partial f}{\partial \eta} \rightarrow 0, \phi \rightarrow 0, g \rightarrow 0, \theta \rightarrow 0 \text{ (as } \eta \rightarrow \infty) \end{aligned} \right\}, \quad (12)$$

3. Physical quantities

Mathematical expressions for Nusselt number and Sherwood number are:

$$\begin{aligned}
C_{fx} &= \frac{\tau_{xr}}{u_w^2 \rho_f}, \quad \tau_{xr} = \mu_f \left(1 + \frac{1}{C_p} + \frac{k}{\mu_f} \right) \frac{\partial u}{\partial r} \Big|_{r=R}, \\
Nu_x &= \frac{xq_w}{k_f (T_w - T_\infty)}, \quad q_w = - \left(k_f + \frac{16\sigma^* T_\infty^3}{3k^*} \right) \left(\frac{\partial T}{\partial r} \right) \Big|_{r=R}, \\
Sh_x &= \frac{xq_m}{D_B (C_w - C_\infty)}, \quad q_m = -D_B \left(\frac{\partial C}{\partial r} \right) \Big|_{r=R},
\end{aligned} \tag{13}$$

Where τ_{xr} and (q_w, q_m) are shear stress and (heat and mass) flux. We have

$$\left. \begin{aligned}
\text{Re}_x^{1/2} C_{fx} &= \left(1 + \frac{1}{C_p} + K \right) f''(0) \\
\text{Re}_x^{-1/2} Nu_x &= - \left(1 + \frac{4}{3} Rd \right) \theta'(0) \\
\text{Re}_x^{-1/2} Sh_x &= -\phi'(0)
\end{aligned} \right\} \quad \text{with} \quad \text{Re}_x = \frac{xu_w}{\nu_f}. \tag{14}$$

4. Solutions

First order and second order truncated solutions are mentioned here.

4.1 Similar solution

For local similar solution we suppose $\frac{\partial(\cdot)}{\partial \xi} = 0$, here $(\xi \ll 1)$. Eqs. (8-12) reduced to

$$\begin{aligned}
&\left(1 + \frac{1}{C_p} + K \right) \left[(1 + 2C\eta) f''' + 2Cf'' \right] + ff'' - (f')^2 - Mf' - K\sqrt{1 + 2C\eta}g' \\
&+ \frac{L}{\xi}(\theta + N\phi) - \left(1 + \frac{1}{C_p} + K \right) P_m f' = 0,
\end{aligned} \tag{15}$$

$$S_g \left[(1 + 2C\eta) g'' + 2Cg' \right] + (1 + 2C\eta) fg' - gf' - (f')^2 - M_p D_p \left(2g + \sqrt{1 + 2C\eta} f'' \right) = 0, \tag{16}$$

$$\begin{aligned}
&\left(1 + \frac{4}{3} R \right) \frac{1}{\text{Pr}} \left((1 + 2C\eta) \theta'' + 2C\theta' \right) + f\theta' + MEc\xi^2 (f')^2 + Q\theta \\
&- \left(1 + \frac{1}{C_p} + K \right) \lambda Ec\xi^2 (f')^2 = 0,
\end{aligned} \tag{17}$$

$$((1+2C\eta)\varphi''+2C\varphi')+Sc(f\varphi'-Cr\varphi)=0, \quad (18)$$

$$\left. \begin{aligned} f' &= 1, f = 0, g = -nf'', \theta' = -A(1-\theta), \varphi' = -B(1-\varphi) \quad (\text{at } \eta = 0) \\ f' &\rightarrow 0, \varphi \rightarrow 0, g \rightarrow 0, \theta \rightarrow 0 \quad (\text{as } \eta \rightarrow \infty) \end{aligned} \right\}, \quad (19)$$

4.2 2nd truncation

Here we introduce new functions $p = \frac{\partial f}{\partial \xi}$, $q = \frac{\partial g}{\partial \xi}$, $r = \frac{\partial \theta}{\partial \xi}$, $s = \frac{\partial \varphi}{\partial \xi}$. Eqs. (8-12) becomes

$$\begin{aligned} &\left(1 + \frac{1}{C_p} + K\right) \left[(1+2C\eta) f''' + 2Cf'' \right] + ff'' - (f')^2 - Mf' - K\sqrt{1+2C\eta}g' \\ &+ \frac{L}{\xi}(\theta + N\varphi) - \left(1 + \frac{1}{C_p} + K\right) P_m f' = -\xi [f''p - f'p'], \end{aligned} \quad (20)$$

$$\begin{aligned} &S_g \left[(1+2C\eta)g'' + 2Cg' \right] + (1+2C\eta)fg' - gf' - (f')^2 \\ &- M_p D_p \left(2g + \sqrt{1+2C\eta}f'' \right) = \xi [f'q - (1+2C\eta)g'p], \end{aligned} \quad (21)$$

$$\begin{aligned} &\left(1 + \frac{4}{3}R\right) \frac{1}{Pr} \left((1+2C\eta)\theta'' + 2C\theta' \right) + f\theta' + MEc\xi^2 (f')^2 + Q\theta \\ &- \left(1 + \frac{1}{C_p} + K\right) \lambda Ec\xi^2 (f')^2 = \xi [rf' - \theta'p], \end{aligned} \quad (22)$$

$$((1+2C\eta)\varphi''+2C\varphi')+Sc(f\varphi-Cr\varphi)=Sc\xi[sf'-\varphi'p], \quad (23)$$

$$\left. \begin{aligned} f' &= 1, f + \xi p = 0, g = -nf'', \theta' = -A(1-\theta), \varphi' = -B(1-\varphi) \quad (\text{at } \eta = 0) \\ f' &\rightarrow 0, \varphi \rightarrow 0, g \rightarrow 0, \theta \rightarrow 0 \quad (\text{as } \eta \rightarrow \infty) \end{aligned} \right\}, \quad (24)$$

Now differentiating Eqs. (20-24) w.r.t ξ and ignoring terms with derivative of ξ . Resultant equations are

$$\begin{aligned} &\left(1 + \frac{1}{C_p} + K\right) \left[(1+2C\eta)p''' + 2Cp'' \right] - 3f'p' + 2pf'' - Mp' + fp'' + K\sqrt{1+2C\eta}q' + \frac{L}{\xi}(r + Ns) \\ &- \frac{L}{\xi^2}(\theta + N\varphi) - \left(1 + \frac{1}{C_p} + K\right) P_m p' - \xi [p'^2 - p''p] = 0, \end{aligned} \quad (25)$$

$$\begin{aligned} &S_g \left[2Cq' + (1+2C\eta)q'' \right] - gp' - 2f'q + (1+2C\eta)(2pg' + fq') \\ &- M_p D_p \left[2q + \sqrt{1+2C\eta}p'' \right] = 0, \end{aligned} \quad (26)$$

$$[2p\theta' + fr' - rf'] + \frac{1}{Pr} \left(1 + \frac{4}{3} R \right) ((1 + 2C\eta)r'' + 2Cr') + 2MEc\xi (f')^2 + 2MEc\xi^2 f' p' + Qr - 2 \left(1 + \frac{1}{C_p} + K \right) P_m Ec \xi f'^2 - 2 \left(1 + \frac{1}{C_p} + K \right) P_m Ec \xi^2 f' p' - \xi [rp' - r'p] = 0, \quad (27)$$

$$((1 + 2C\eta)s'' + 2Cs') + (2p\phi' + fs' - sCr - sf')Sc = Sc\xi [p's - ps'], \quad (28)$$

$$\left. \begin{aligned} p' = 0, \quad p = 0, \quad q = -\eta f'', \quad r' = -Ar, \quad s' = -sB \quad (\text{at } \eta = 0) \\ p' \rightarrow 0, \quad q \rightarrow 0, \quad r \rightarrow 0, \quad s \rightarrow 0 \quad (\text{as } \eta \rightarrow \infty) \end{aligned} \right\}, \quad (29)$$

5. Solution Methodology

Step by step methodology is mentioned in following flow chart.

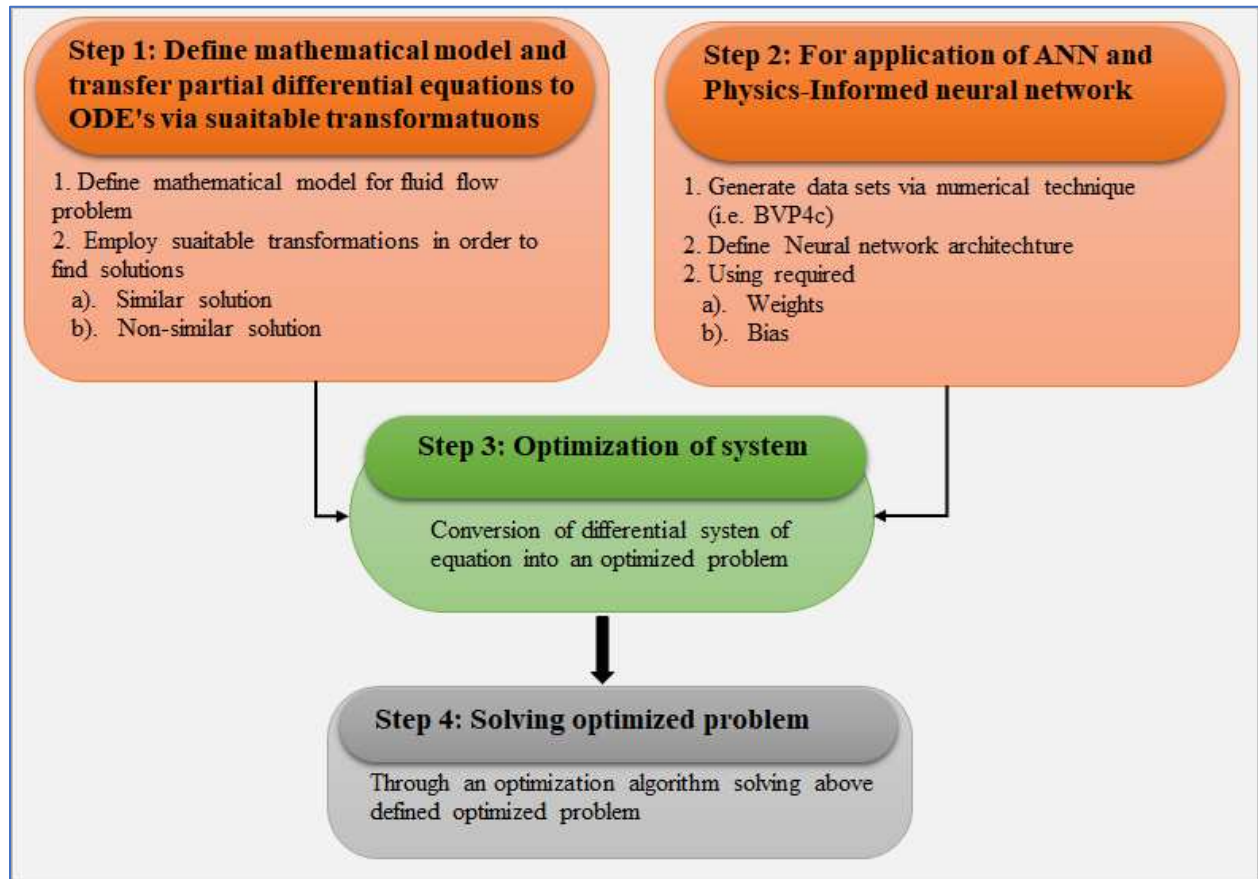


Fig. 2: Flow chart.

5.1 Physics Informed Neural Network

Physics-informed Neural Network gives a data-driven computational and mesh independent technique which offers physical principles for loss function of neural network. Here **Fig. 3** explains step by step procedure of PINN approach.

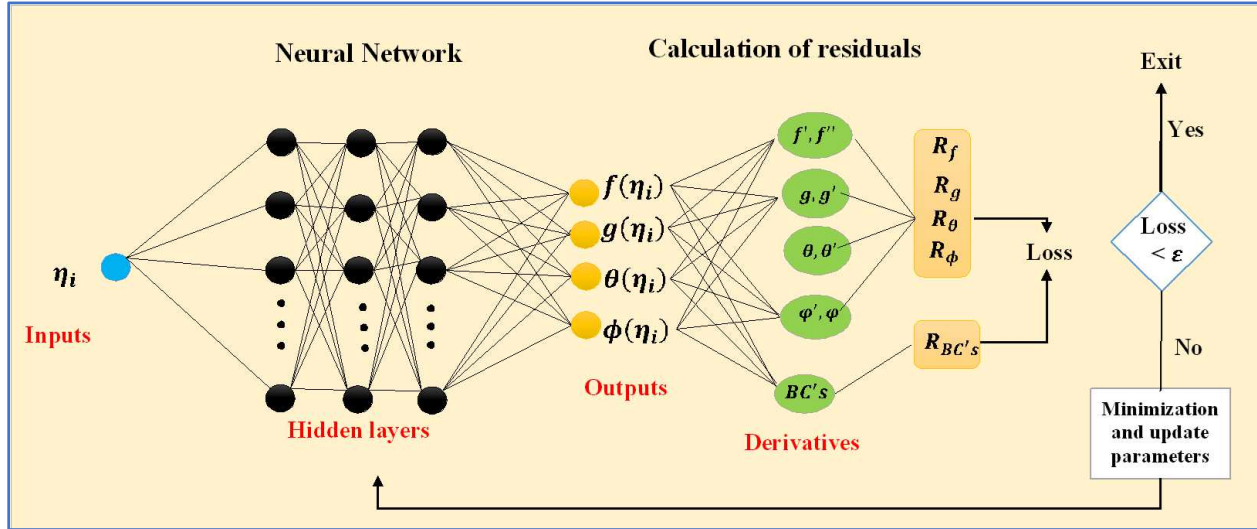


Fig. 3: PINN Architecture.

Network Architecture in **Fig. 3** depicts the inputs η_i fed to the network. The first layer, such as the input layer having a single neuron holding fed data. The output layer having (3) neurons with same number of hidden layers. All neurons are attached via links with weight w_{ij} . This weight either enhances or decreases the amount of information passing from the source to destination neuron. Weight evaluates the contribution of each neuron in producing an outcome in the output neurons:

$$z_i = \sum_{j=1}^{j=n} a_j \cdot w_{i,j}^k + b_j, \quad (30)$$

Applied activation function with (z_i) fed

$$Output(i) = \tanh(z_i) \quad (31)$$

In this system there are momentum, heat and mass loss functions involved with loss function of taken boundaries. These loss functions are defined as:

$$L_{physics} = \frac{1}{N} \sum_{i=1}^N \left[\begin{aligned} & \left\{ \left(1 + \frac{1}{C_p} + K \right) \left[(1 + 2C\eta) f''' + 2Cf'' \right] + ff'' - (f')^2 \right\}^2 \\ & \left\{ -Mf' - K\sqrt{1+2C\eta}g' + \frac{L}{\xi}(\theta + N\varphi) - \left(1 + \frac{1}{C_p} + K \right) P_m f' \right\}^2 \\ & \left\{ S_g \left[(1 + 2C\eta) g'' + 2Cg' \right] + (1 + 2C\eta) fg' - gf' - (f')^2 \right\}^2 \\ & \left\{ -M_p D_p (2g + \sqrt{1+2C\eta}f'') \right\}^2 \\ & \left\{ \left(1 + \frac{4}{3}R \right) \frac{1}{Pr} \left((1 + 2C\eta)\theta'' + 2C\theta' \right) + f\theta' + MEc\xi^2 (f')^2 \right\}^2 \\ & \left\{ +Q\theta - \left(1 + \frac{1}{C_p} + K \right) \lambda Ec\xi^2 (f')^2 \right\}^2 \\ & + \left\{ ((1 + 2C\eta)\varphi'' + 2C\varphi') + Sc(f\varphi' - C\varphi) \right\}^2 \end{aligned} \right], \quad (32)$$

Boundary conditions loss can be defined as:

$$L_{BC's} = \frac{1}{N} \sum_{i=1}^N \left[\begin{aligned} & \left\{ f(0) \right\}^2 + \left\{ f'(0) - 1 \right\}^2 + \left\{ f'(\infty) \right\}^2 + \left\{ g(0) + nf''(0) \right\}^2 + \left\{ g(\infty) \right\}^2 \\ & + \left\{ \theta'(0) + A(1 - \theta(0)) \right\}^2 + \left\{ \theta(\infty) \right\}^2 + \left\{ \varphi'(0) + A(1 - \varphi(0)) \right\}^2 + \left\{ \varphi(\infty) \right\}^2 \end{aligned} \right], \quad (33)$$

Then the total loss can be calculated as:

$$Total \ Loss = L_{data} + L_{physics} + L_{BC's}. \quad (34)$$

6. Results and Discussion

Here we will discuss graphical and numerical results. We'll also perform a comparison of numerical technique i.e. BVP4c with ANN and a stochastic approach Physics-informed neural network (PINN) for f' , g , θ and φ .

6.1 Comparison of BVP4c and PINN at various epochs threshold

Here we perform a comparison study between a numerical technique (i.e. BVP4c) and a stochastic neural network named as Physics-informed neural network at different stages of iterations for all considered profiles i.e. velocity, microrotation, thermal and mass. At (1000)–epochs, Fig. 4(a) clears that network fails to sort out boundary layer dynamics. Here predicted curves for velocity, microrotation, temperature and mass deviate numerically plotted curves. It signifies weak approximation because of insufficient training epochs. At (20,000)–epochs, Fig. 5(a) demonstrates that PINN model generates highly accurate results and consistent with BVP4c

reference outcomes. This progression confirms that with high number of iterations ability of network to resolve complex problems is improved with a fast convergence to benchmark solutions.

6.2 Convergence of Developed PINN Scheme Using Loss Function

Computational effectiveness and mathematical reliability of PINN model analyzed via convergence characteristics behavior with its composite loss function over considered number of epochs. Loss function defined in Eq. (34) is used for optimization, it simultaneously reduces residuals corresponding to momentum, microrotation, heat and mass equations with prescribed boundary constraints. As number of iterations increases loss function shows a decreasing behavior, it reflects smooth stability and fast convergence of network parameters. Gradually total function reduces; it indicates a good correlation between numerical reference outcomes and PINN predictions with a great accuracy and smoothness that guarantees fast convergence.

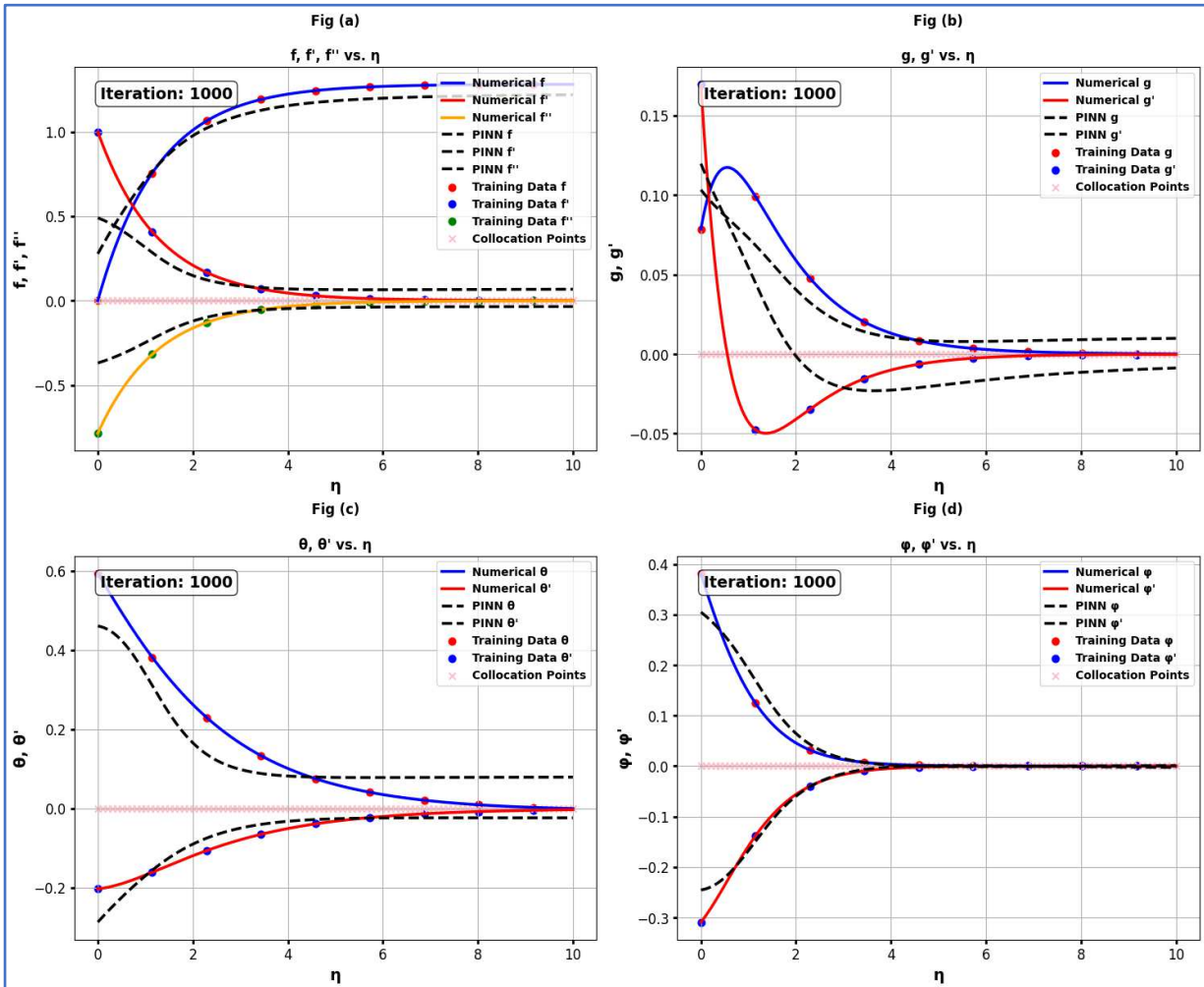


Fig. 4(a): At (1000) – epochs PINN and BVP4c results comparison.

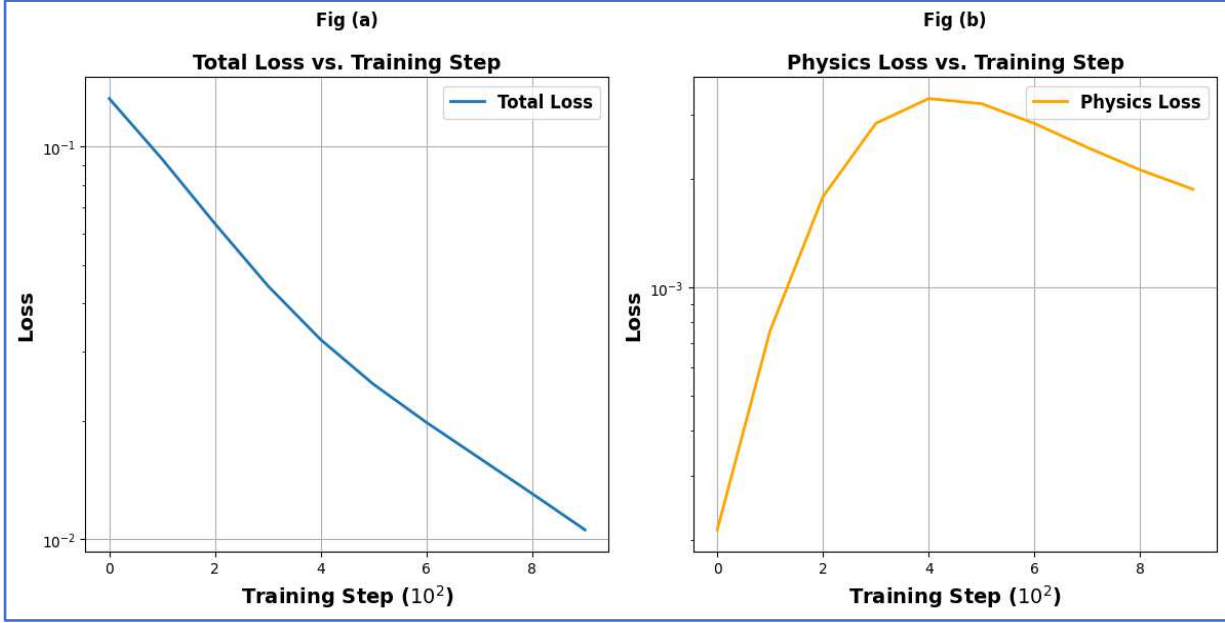


Fig. 4(b): At (1000)–epochs convergence of PINN algorithms via loss function.

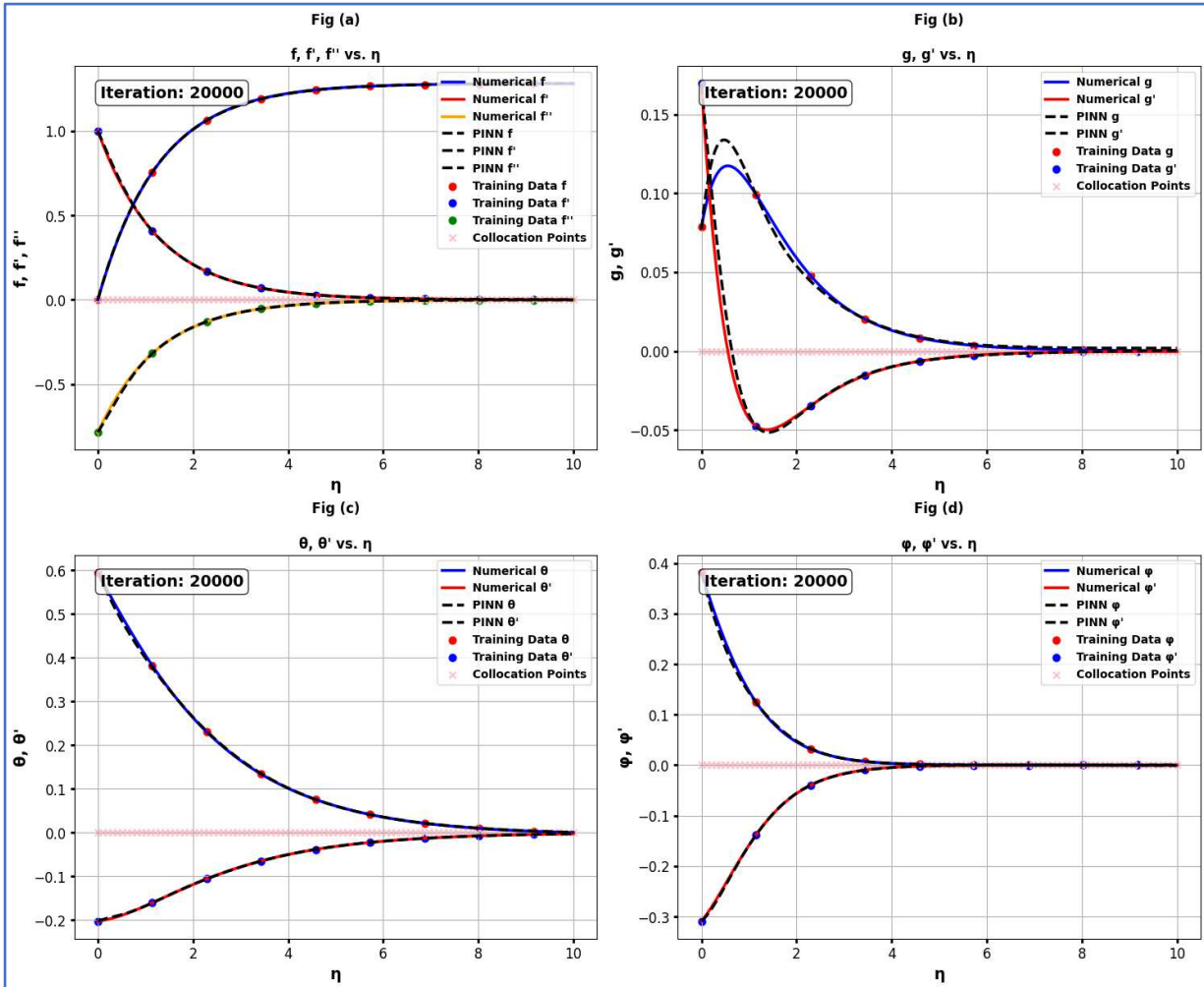


Fig. 5(a): At (20000) – epochs PINN and BVP4c results comparison.

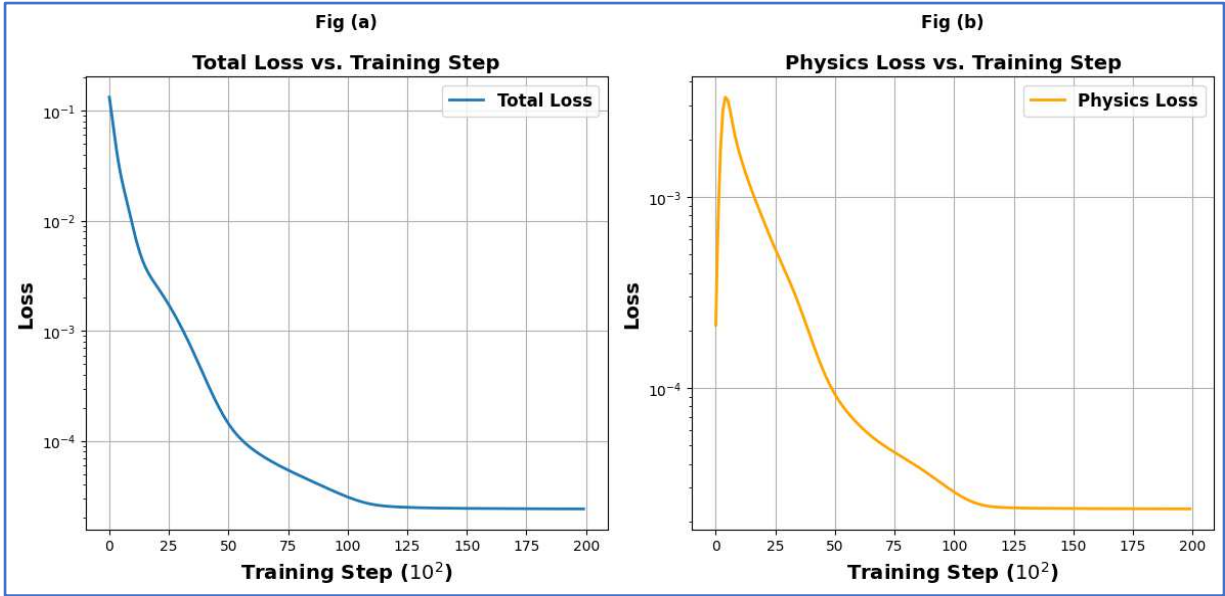


Fig. 5(b): At (20000) – epochs convergence of PINN algorithms via loss function.

6.3 Mean absolute error (MAE)

Mean absolute error (MAE) is basically a difference between predicted values via PINN/ANN and reference data (Numerical solution). With very small MAE values one can conclude that proposed model has high authenticity and fast convergence. **Table 1** and **2** are built for comparison of mean absolute error analysis at different number of epochs. It is clear from table that as we increase number of epochs from 1000 to 20,000 means absolute error corresponding to all dependent variables as well as their corresponding derivatives decreases, it indicates a continuous improvement in model's learning ability and convergence. Markedly lowest mean absolute errors are obtained at 20,000 epochs confirms model's enhanced predictivity, authenticity, effectiveness and numerical stability.

Table 1: Mean absolute error at (1000) – epochs.

Variable	Mean absolute error
f	0.001086
f'	0.000983
f''	0.001319
g	0.002506
g'	0.001592
θ	0.001504
θ'	0.000262
ϕ	0.001210

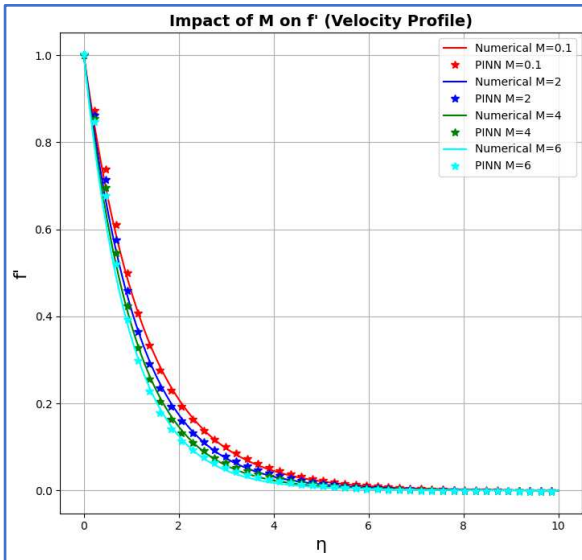
Variable	Mean absolute error
f	0.065183
f'	0.076594
f''	0.051274
g	0.010681
g'	0.023538
θ	0.060227
θ'	0.018359
ϕ	0.008205
ϕ'	0.004468

ϕ'	0.000500
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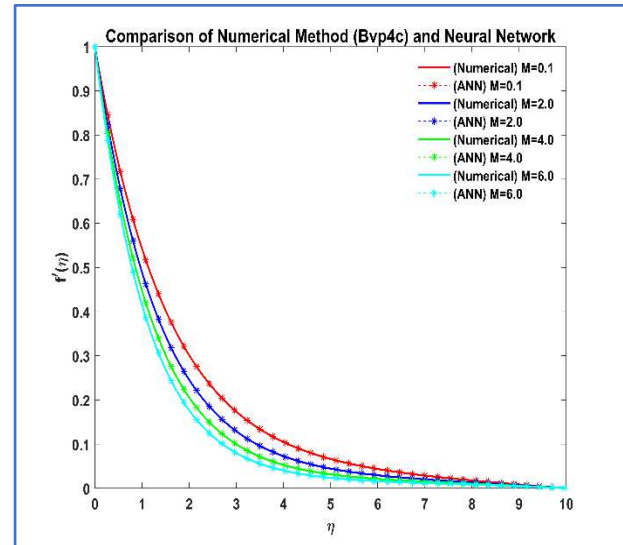
Table 2: Mean absolute error at (20000)–epochs.

6.4 Velocity behavior

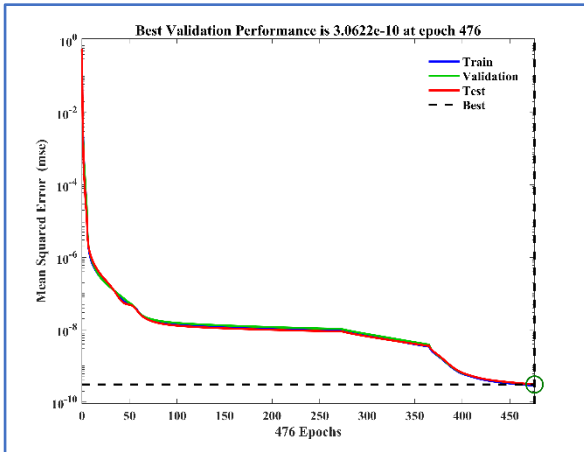
Figs. 6(a-g) shows a comparative analysis of numerical technique and Machine learning approaches (i.e. ANN and PINN). This comparative analysis demonstrates an excellent agreement between (PINN and ANN) with BVP4c solutions for velocity versus magnetic strength, it sures predictive and robustness ability of considered proposed neural network models. Clearly against strong magnetic strength velocity of fluid suppresses, it reflects that as we enhance magnetic field Lorentz force augmented that opposes motion of fluid, consequently momentum profile suppresses. Training performance further validating networks stability by achieving a very small mean square error ($3.0622e^{-10}$) at 476 iterations. It is accompanied by smooth convergence of gradient, ignorable validation checks and error distributions around zero. Further, regression analysis and fitness functions plots display an excellent correlation ($R=1$) between network's outputs and target data for training, testing and validation data subsets, it ensures good learning authenticity and excellent generalization capability of neural network.



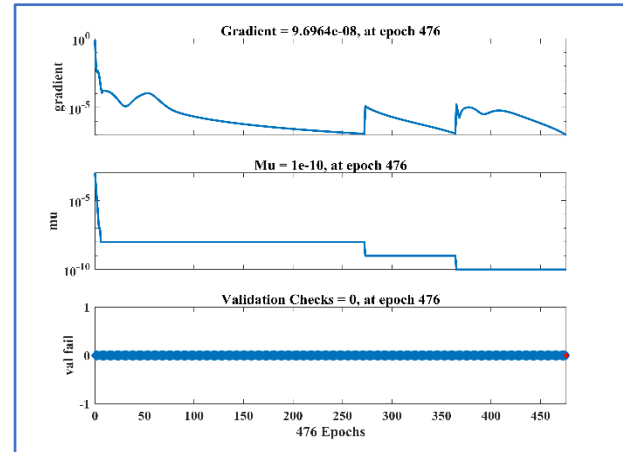
(a)



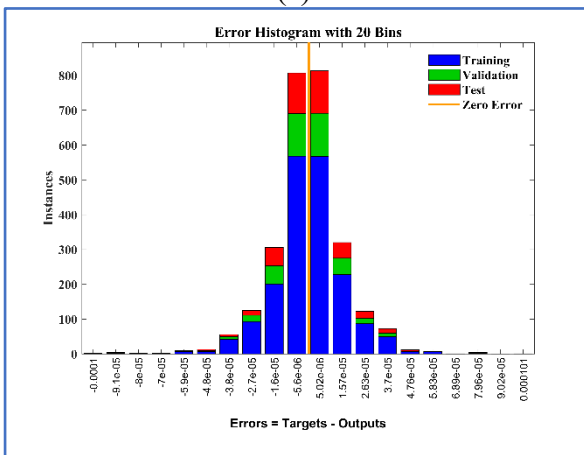
(b)



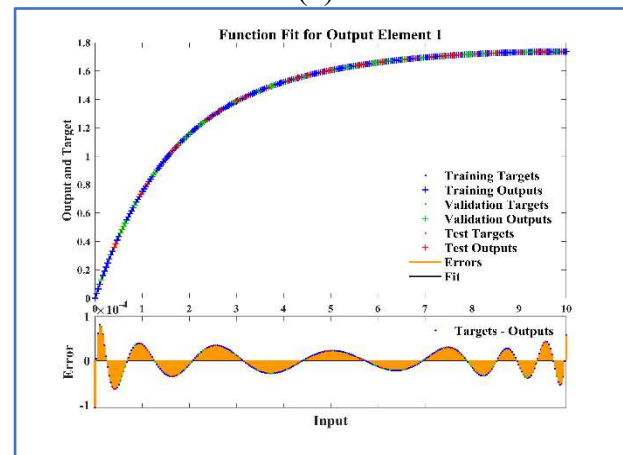
(c)



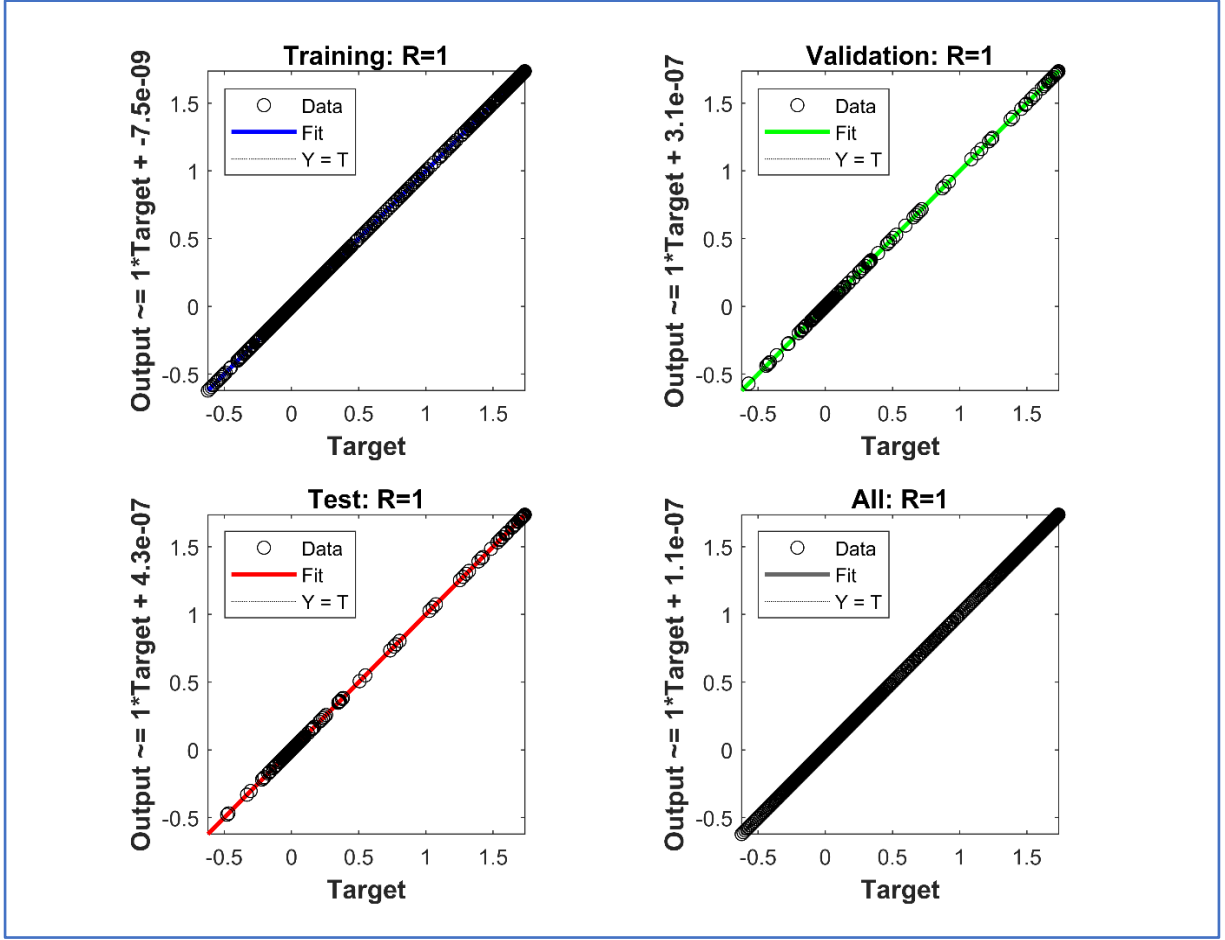
(d)



(e)



(f)



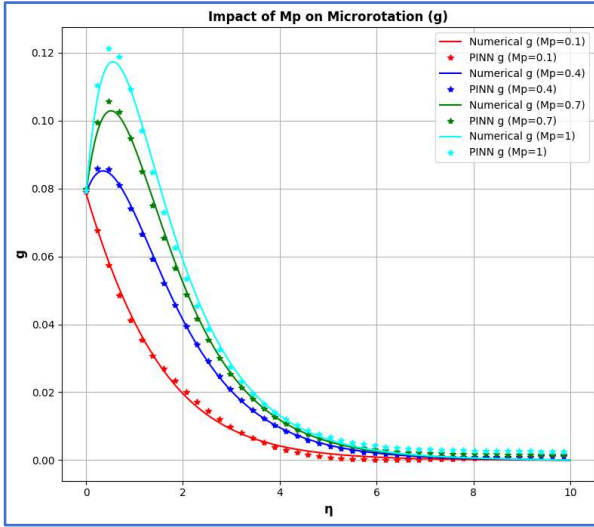
(g)

Fig. 6(a-g): Bvp4c comparison with ANN and PINN outcomes of velocity profile against M , (a) PINN vs BVP4c (b) ANN vs BVP4c (c) MSE (d) Gradient state (e) EH (f) Fitness function and (g) Regression analysis.

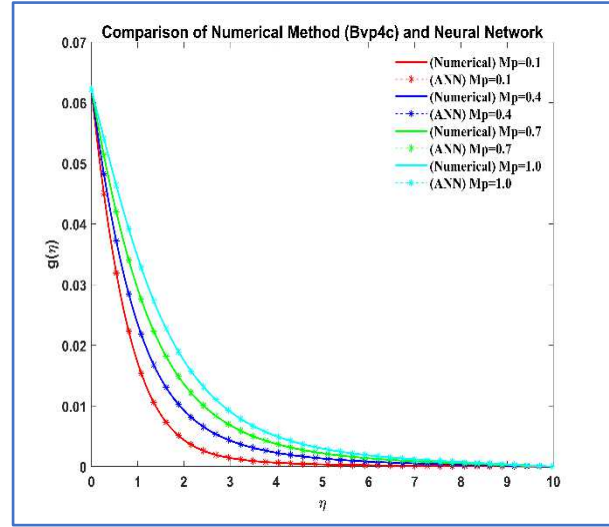
6.5 Microrotation

Fig. 7(a-g) shows a comprehensive analysis of formulated neural networks in order to predict micro-rotational profile against micropolar parameters. **Figs. 7(a)** and **(b)** display that BVP4c's reference solutions exhibit an excellent agreement with prediction generated via ANN and PINN models, it confirms highly accurate predictions of proposed models. Higher values of M_p results in an increase of micro-rotational profile, which demonstrates stronger rotational behavior of (micro-structured) fluid particles. Neural network's numerical stability is demonstrated by smallest MSE value i.e. $(1.1242e^{-09})$ at epochs 527, similarly collectively (μ) i.e. adaptive parameter, gradient and validation checks guarantee fast and smooth convergence without instability of optimization. Here error plots in histograms display a narrow distribution around zero-error line, likewise fitness plot along regression analysis ($R=1$) guarantees a perfect correlation between all datasets. Here one can conclude that formulated neural network approaches

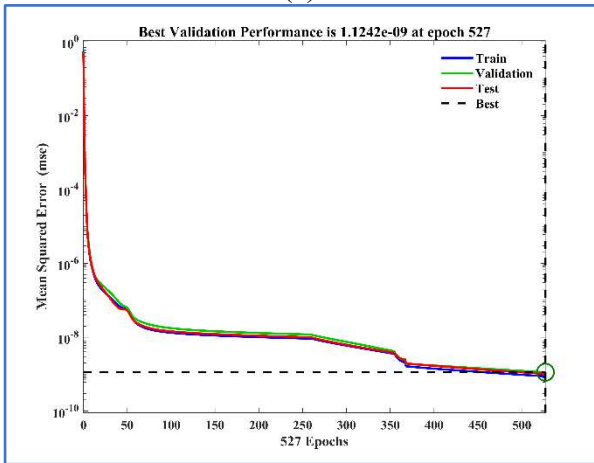
give accurate, robust and computationally effective solutions except from convectional numerical techniques (i.e. BVP4c).



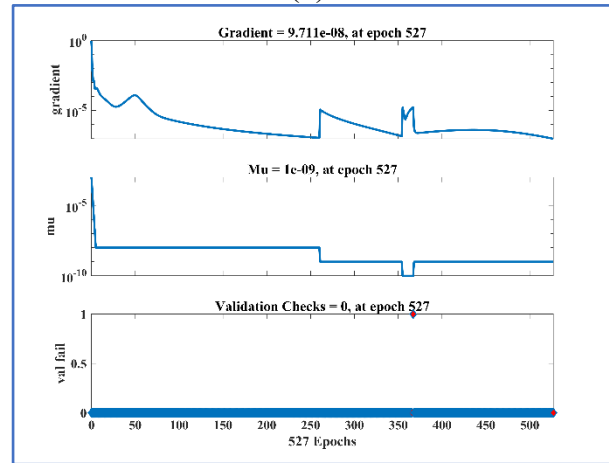
(a)



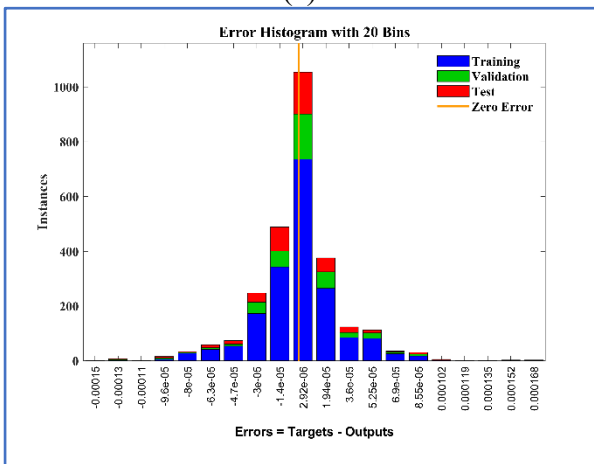
(b)



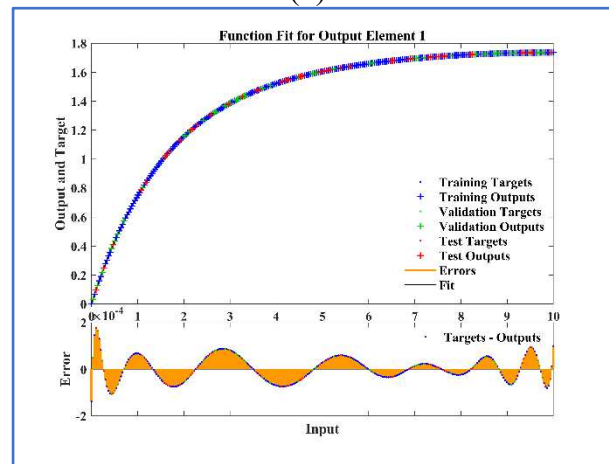
(c)



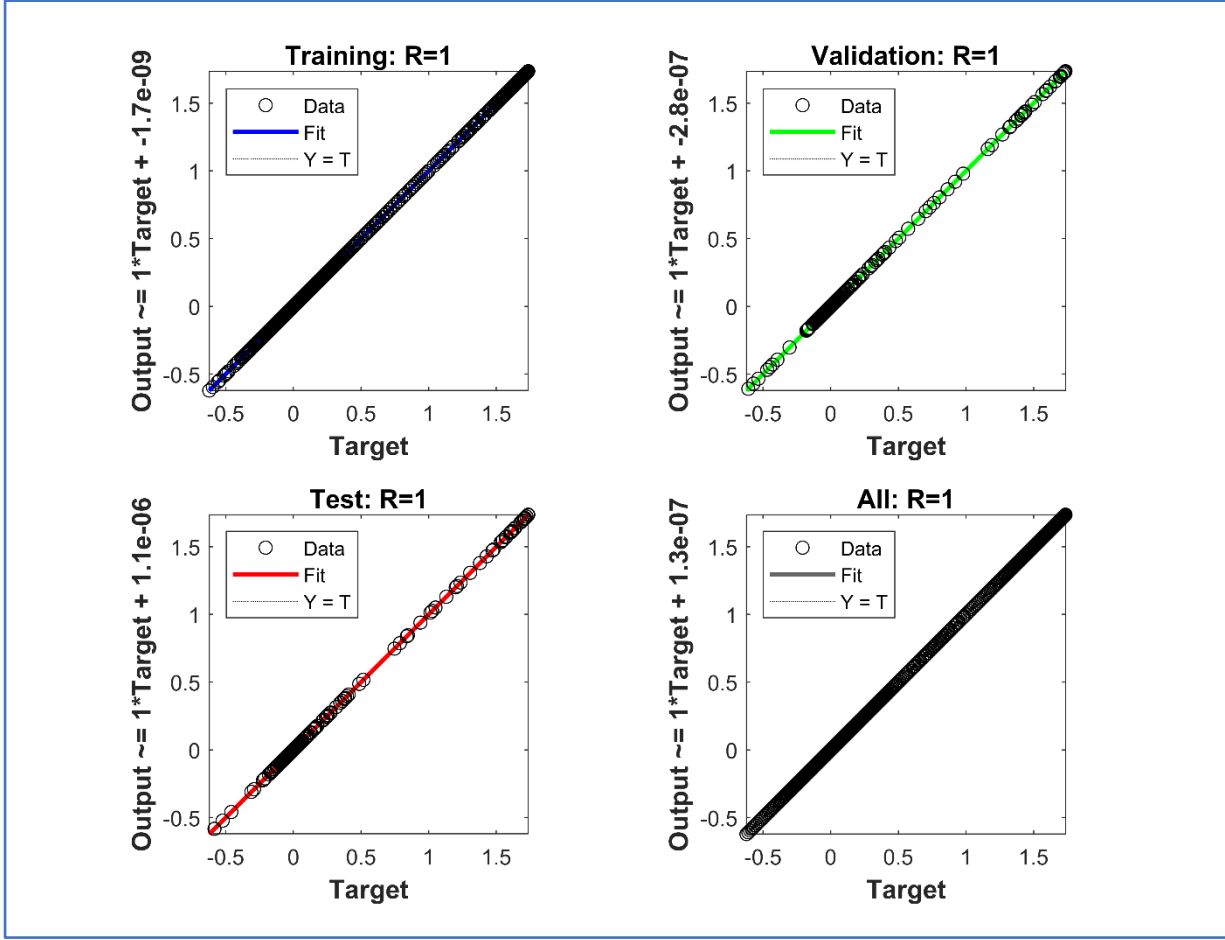
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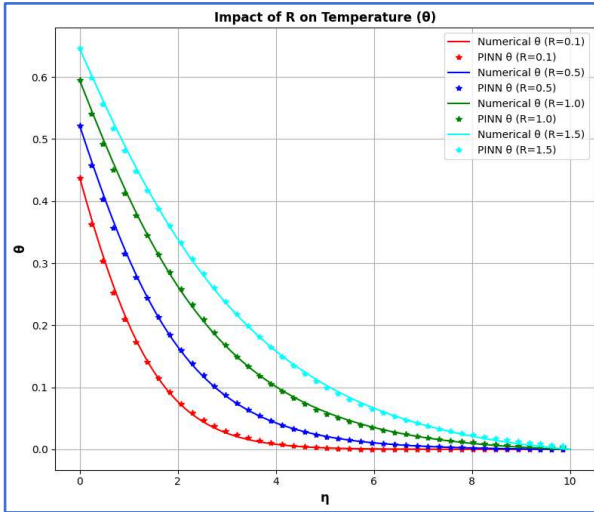
(g)

Fig. 7(a-g): Bvp4c comparison with ANN and PINN outcomes of microrotation profile against M_p , (a) PINN vs BVP4c (b) ANN vs BVP4c (c) MSE (d) Gradient state (e) EH (f) Fitness function and (g) Regression analysis.

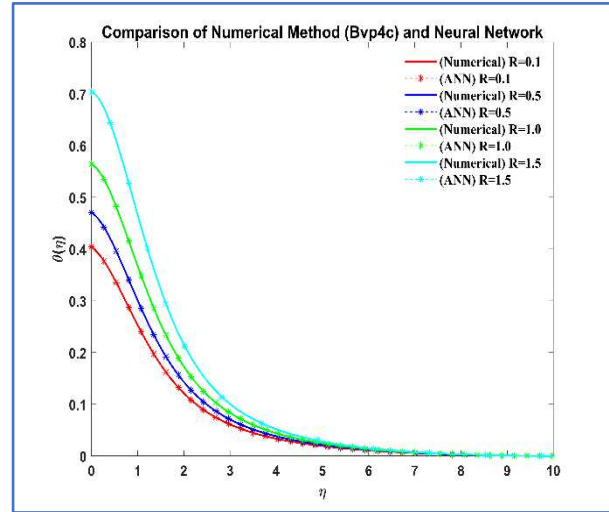
6.6 Temperature

Fig. 8(a-g) displays a complete analysis of thermal profile against thermal radiation along performance evaluation of formulated models of neural network. **Fig. 8(a)** and **(b)** analyze BVP4c's solutions as reference data along predictions generated via PINN and ANN against radiation parameters. An excellent agreement between ANN, PINN and reference solutions generated via BVP4c sures authenticity and consistency of proposed models. It is understood that as we increase thermal radiation parameters consequently temperature of fluid increases accordingly. **Fig. 8(c)** and **(d)** demonstrates efficient and stable network optimization having lowest MSE numerical value i.e. $(4.8022e^{-09})$ at 510 epochs, likewise, zero validation failures, adaptive damping number and gradient evaluation verify smooth and consistent convergence with zero instability. Furthermore, EH guarantees that errors in predictions are strongly clustered around zero-error line. Regression plots and function fitness analysis having correlation coefficient

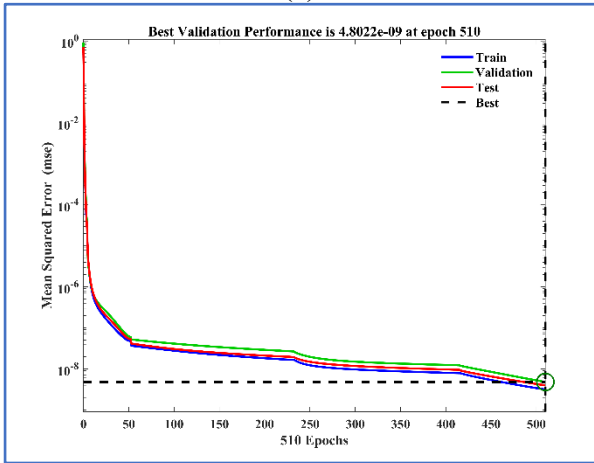
$R=1$, which indicates perfect correlation for complete datasets. Thus, it can be concluded that proposed models are reliable, robust and authentic with minimum error ratio in order to get predictions against physical parameters.



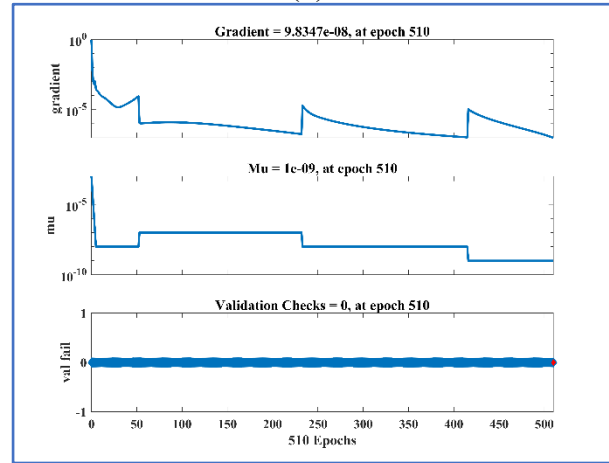
(a)



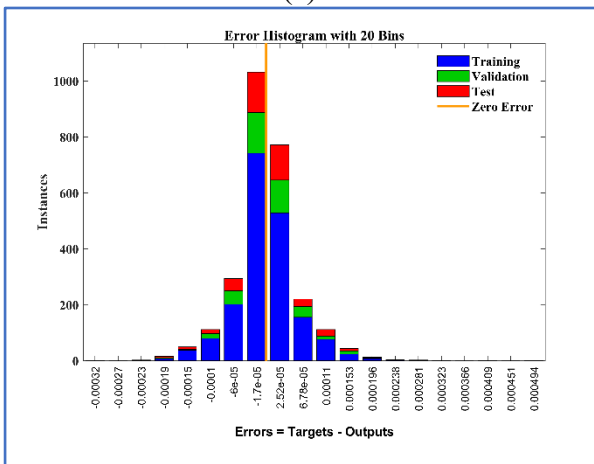
(b)



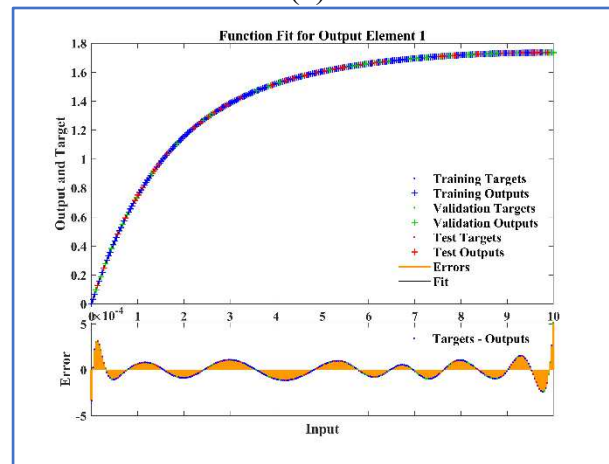
(c)



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(f)

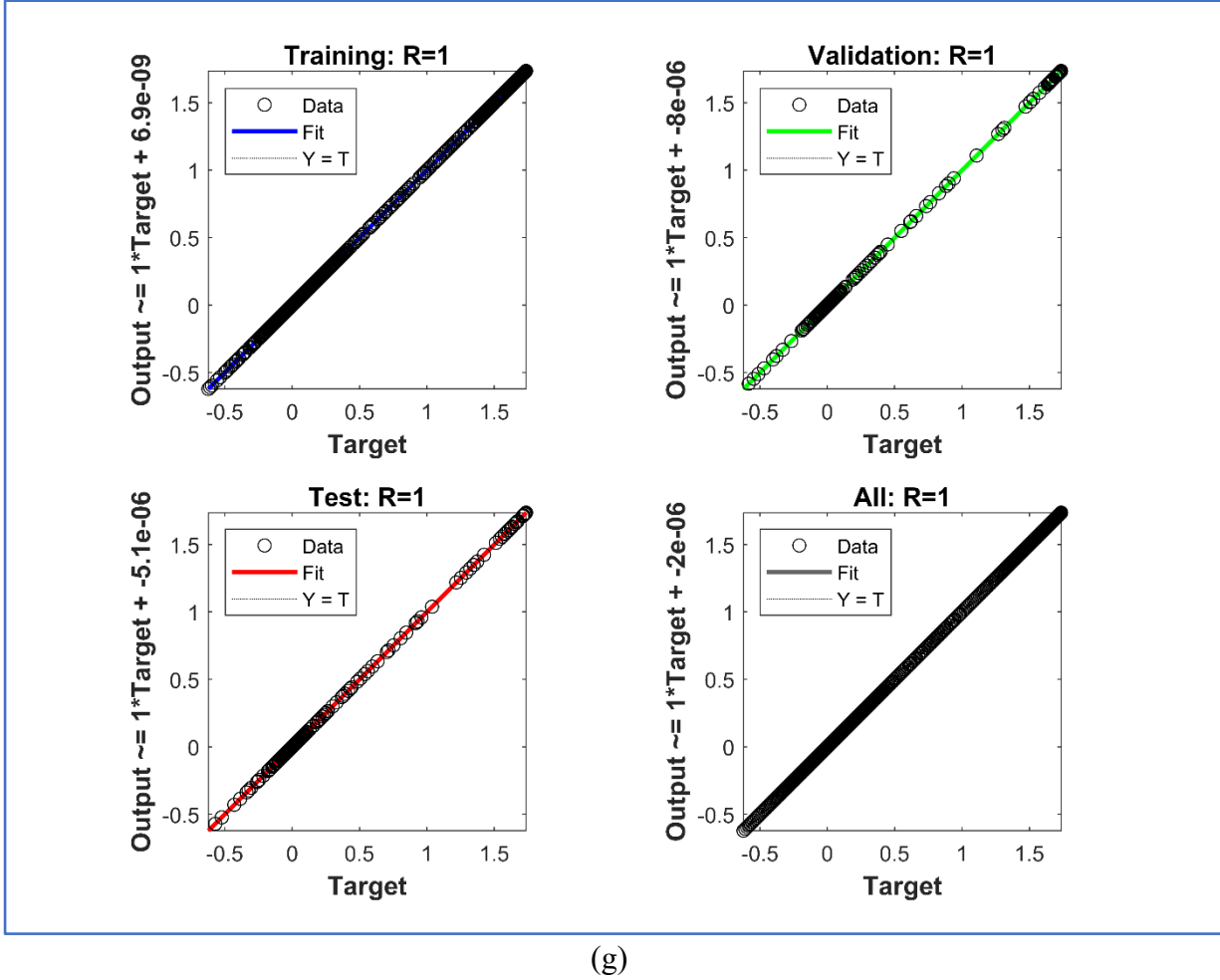
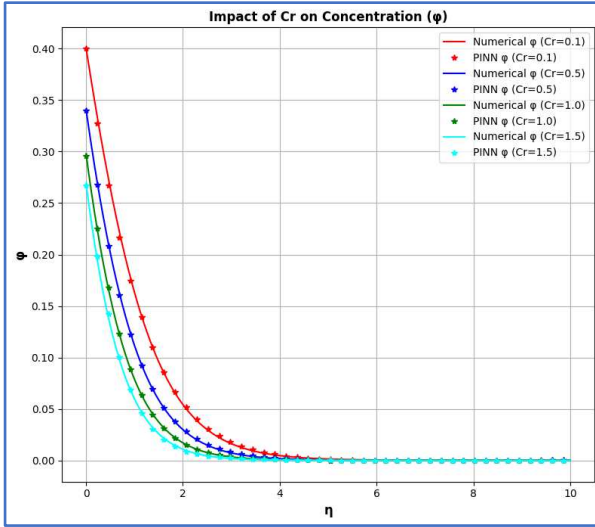


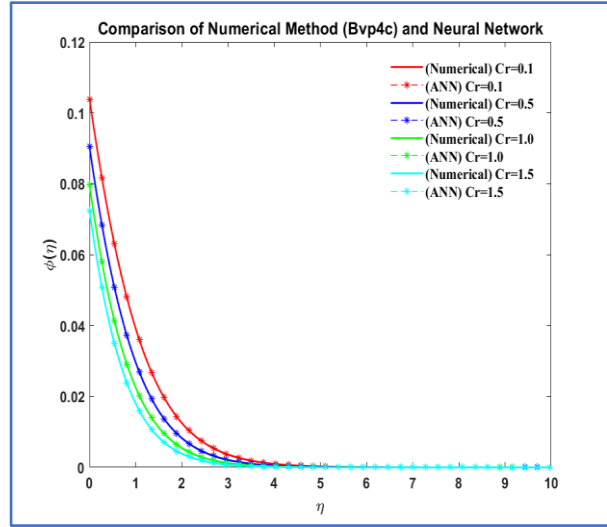
Fig. 8(a-g): Bvp4c comparison with ANN and PINN outcomes of thermal profile against R , (a) PINN vs BVP4c (b) ANN vs BVP4c (c) MSE (d) Gradient state (e) EH (f) Fitness function and (g) Regression analysis.

6.7 Concentration

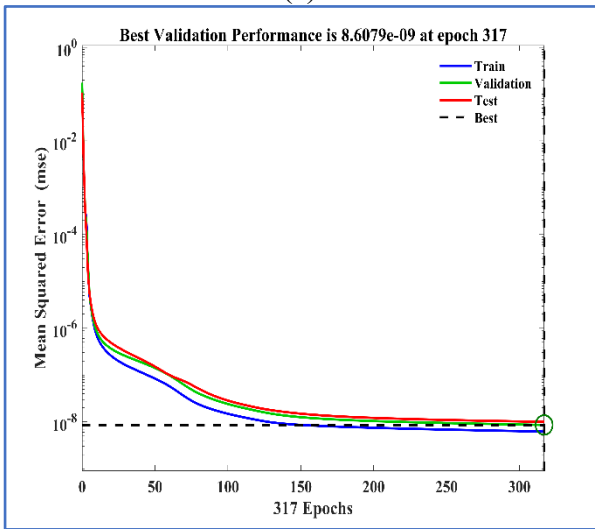
Fig. 9(a-g) displays a comprehensive graphical overview of proposed model's (i.e. PINN and ANN) against reference solutions generated via a famous numerical technique (i.e. BVP4c) for mass profile against Cr . **Fig. 9(a)** and **(b)** display an excellent consensus between PINN/ANN predictions and reference plots for various number of chemical reaction parameters. It confirms authenticity and reliability of developed neural networks for computational analysis. One can conclude that enhanced species consumption due to strongest chemical reaction mass profile shrinks. Small MSE value i.e. $(8.6079e^{-09})$ at 317 epochs, obtained during network training indicates fast convergence and stability of model, while zero validation checks and gradient analysis indicate robust optimization. Errors in predictive results are clustered around zero error line indicating minimum errors. Similarly, regression and fitness plots display good correlation between all sub-datasets with no overfitting. From this analysis one can conclude that proposed neural networks are accurate and stable for computational results as an alternative approach.



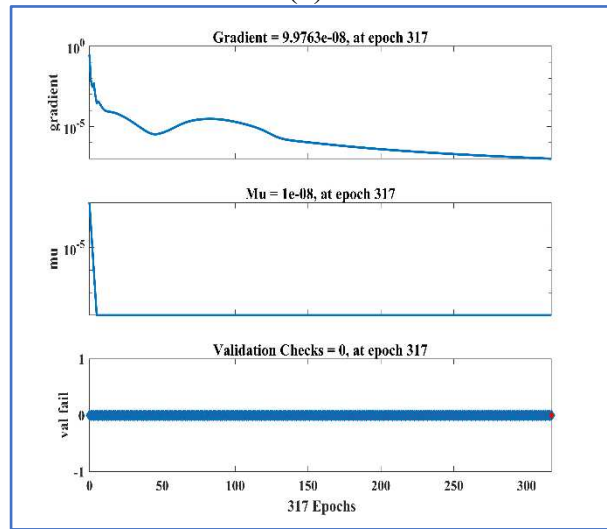
(a)



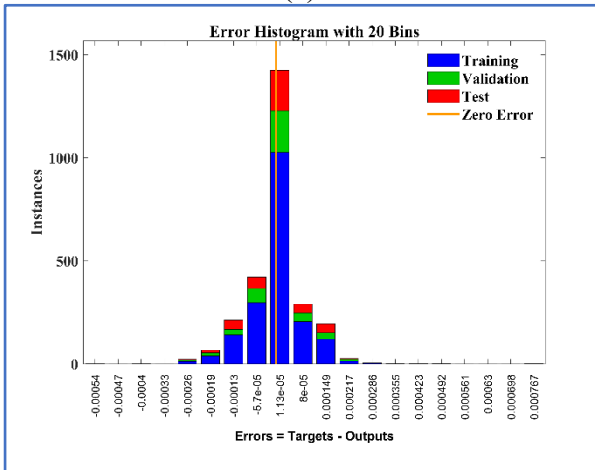
(b)



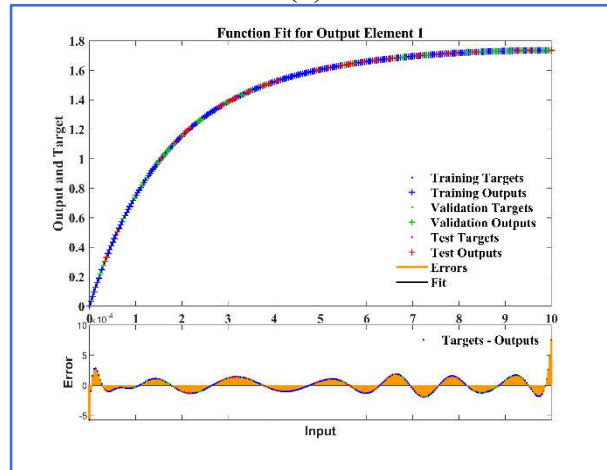
(c)



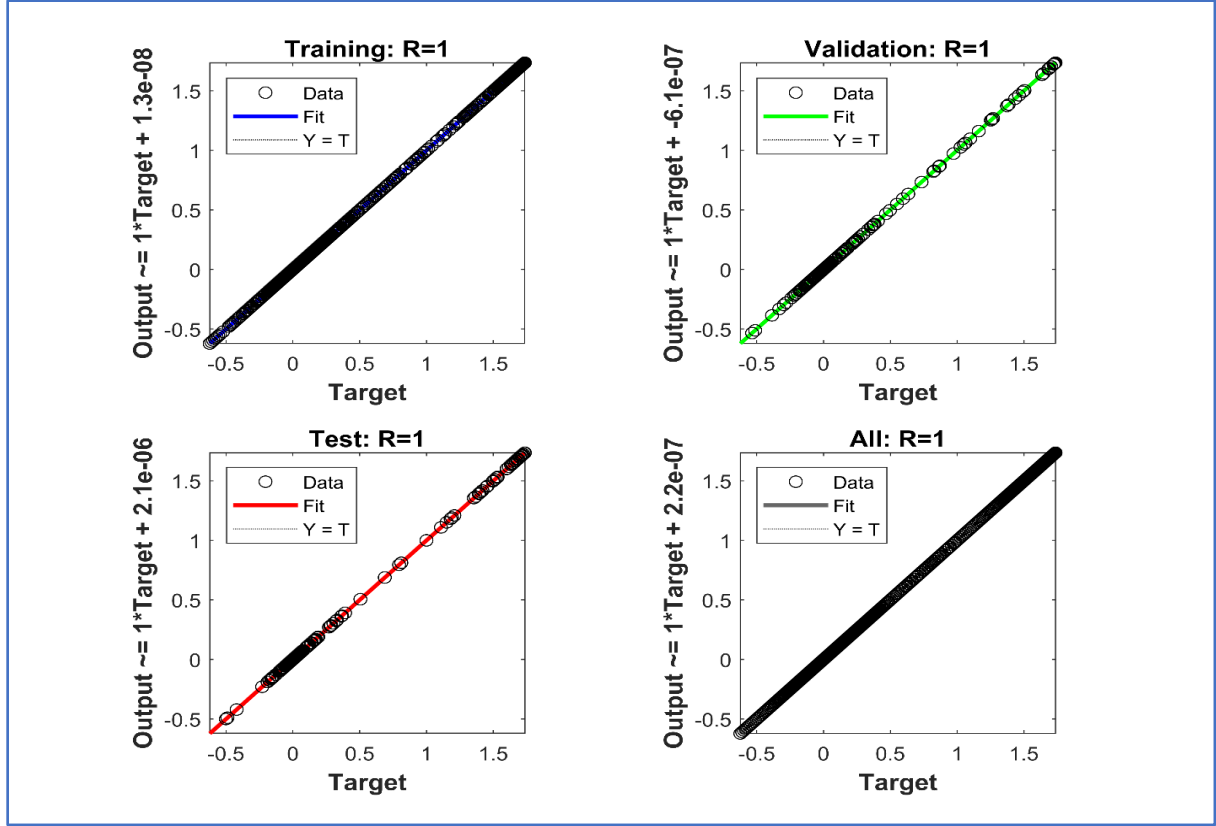
(d)



(e)



(f)



(g)

Fig. 9(a-g): Bvp4c comparison with ANN and PINN outcomes of mass profile against Cr (a) PINN vs BVP4c (b) ANN vs BVP4c (c) MSE (d) Gradient state (e) EH (f) Fitness function and (g) Regression analysis.

7. Final remarks

In present study we proposed neural network models i.e. Physics-Informed and artificial Neural Networks in order to simulate heat, microrotation, mass and velocity outcomes compared with a numerical technique (i.e. BVP4c).

- Higher magnetic strength caused a suppression in fluid's velocity. At (20,000) iteration PINN and numerical results overlap indicating accuracy of proposed network.
- (Mp and R) having direct impact on micro-rotation and thermal field but chemical reaction and mass profile both are inversely proportional to each other.
- For higher number of epochs mean absolute error decreases, i.e. from (1000–20,000) epochs MAE decays from $(10^{-01} - 10^{-02})$ to $(10^{-03} - 10^{-04})$. It ensures proposed model's predictivity accuracy.
- For f' , θ , g and ϕ against physical parameters (M , R , Mp , Cr) respectively, shows stable and accurate solutions as number of epochs increases.

- Formulated neural networks give highly accurate, stable and computationally reliable approach alternate to numerical techniques for nonlinear system of equations.

Nomenclature

u_o	Reference velocity	$P_m \left(= \frac{l\mu_f}{ku_o\rho_f} \right)$	Permeability parameter
(x, r)	Cartesian coordinates (m)	$Q \left(= \frac{lQ_0}{(\rho c_p)_f u_o} \right)$	Heat generation\absorption parameter
σ_f	Electrical conductivity	Q_o	Heat source coefficient
C_b	Coefficient of drag force	$S_g \left(= \frac{\gamma}{\rho_f J v_f} \right)$	Spin gradient parameter
ρ_f	Density (kgm^{-3})	c_p	Specific heat
μ_f	Dynamic viscosity (m^2s^{-1})	M_o	Magnetic field strength
$u_w \left(= \frac{u_o}{l} x \right)$	Stretching velocity	$Sc \left(= \frac{v_f}{D_B} \right)$	Schmidt number
k_f	Thermal diffusivity ($kgms^{-3}K^{-1}$)	$C \left(= \sqrt{\frac{lv_f}{u_o R^2}} \right)$	Curvature parameter
D_B	Brownian diffusion	k_p	Permeability of porous media
C_w^*	Wall concentration	C_{fx}	Wall shear stress
T	Temperature (K)	$R \left(= \frac{4\sigma^* T_\infty^3}{k_f k^*} \right)$	Radiation parameter
(A, B)	Thermal and Solutal Biot number	(h_f, h_w)	Heat and mass transfer rates
Sh_x	Sherwood number	$Pr \left(= \frac{v_f(\rho c_p)_f}{k_f} \right)$	Prandtl number
(u, v)	Velocity components (ms^{-1})	$M \left(= \frac{l\sigma_f B_0^2}{u_o \rho_f} \right)$	Magnetic field parameter
Nu_x	Nusselt number	T_w	Wall temperature
$M_p \left(= \frac{k}{\rho_f J v_f} \right)$	Micro-coupling parameter	$D_p \left(= \frac{lv_f}{u_o} \right)$	Micro-inertia parameter

l	Reference length	$Cr \left(= \frac{lk_r}{u_o} \right)$	Reaction rate
C_p	Casson fluid parameter	k^*	Mean absorption coefficient
γ	Spin gradient viscosity	J	Micro-inertia densirt
k_r	Reaction rate	$Ec = \frac{u_o^2}{c_p (T_w - T_\infty)}$	Eckert number
T_∞	Ambient temperature	$\phi(\eta)$	Concentration (dimensionless)
$A \left(= \frac{h_f}{k_f} \sqrt{\frac{l\nu_f}{u_o}} \right)$	Thermal Biot number	$B \left(= \frac{h_w}{D_B} \sqrt{\frac{l\nu_f}{u_o}} \right)$	Solutal Biot number
ν_f	Kinematic viscosity (m^2s^{-1})	σ^*	Stefan-Boltzman constant ($Wm^{-2}k^{-4}$)

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