Fourth order Predictor-Corrector Method (PC4-FDM)

UNDERGRADUATE THESIS

Submitted in partial fulfillment of the requirements of
BITS F422T Thesis

By

Lavina CHOTRANI
ID No. 2016B4A80194P

Under the supervision of:

Dr. Bhupendra KUMAR SHARMA

BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE PILANI, PILANI CAMPUS
May 2021

Certificate

This is to certify that the thesis entitled, "*Fourth order Predictor-Corrector Method (PC4-FDM)*" and submitted by Lavina CHOTRANI ID No. 2016B4A80194P in partial fulfillment of the requirements of BITS F422T Thesis embodies the work done by her under my supervision.

Supervisor
Dr. Bhupendra KUMAR SHARMA
Faculty,
BITS-Pilani Pilani Campus
Date:

BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE PILANI, PILANI CAMPUS

Abstract

Master of Science (Hons.)

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by Lavina CHOTRANI

One of the major reasons for carrying out this research is to analyze the effect of a non-uniform heat source or sink along with thermal radiation on the flow of an unsteady MHD Micropolar fluid over a stretching or shrinking sheet. We firstly take into account an already existing research by M.M. Khader and Ram Prakash Sharma wherein they transform the governing non-linear PDEs which were obtained from Eringen's theory for Micropolar fluids into a system of non-linear coupled ODEs which are then solved numerically by using the fourth order predictor–corrector finite difference method (PC4-FDM). The major aspect of this paper is to understand the implementation of the above process and later come up with alternate approaches to further optimize the results obtained and move towards the solution of the non-linear PDEs.

Acknowledgements

First of all, I am extremely thankful to Birla Institute of Technology Science and its Thesis program in particular the Dean, Academic-Undergraduate Studies Division for giving me the opportunity to do the project. This project wouldn't have reached the current progress without the constant support and backing of the Department of Mathematics, BITS Pilani.

Further I would like to express my deepest gratitude to Dr. Bhupendra Kumar Sharma, for consenting to do this thesis under him and for the constant guidance and support throughout this project. I would like to sincerely thank Miss. Rishu Gandhi, Research Scholar from the Mathematics Department for the constant encouragement and insightful direction for all those times that the project seemed to have been stuck.

Lastly, I express thanks to all the people I know from BITS Pilani, friends and otherwise who have encouraged me from time to time, and helped me remain motivated towards the completion of this project.

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Abbreviations

LAH	**L**ist **A**bbreviations **H**ere
MHD	**M**agneto- **H**ydro **D**ynamics
Re	**R**eynolds Number
λ	Stretching/shrinking Parameter
C_p	Specific Heat at Constant Pressure
C_w	Concentration of the solute at the sheet
C_∞	Concentration of the solute far from the sheet
K	Kinematic micro-rotation viscosity
N	Micro-rotation component
β	Coefficient of thermal expansion
β^*	Coefficient of concentration expansion
μ	Coefficient of viscosity
ρ	Fluid Density
T_w	Temperature of the fluid
T_∞	Concentration of the solute far from the sheet
α	Stretching rate
σ	Electrical conductivity
γ	Spin gradient viscosity
j	Micro-inertia density
q_r	Radiative heat flow
D_m	Molecular Diffusivity
$q^{'''}$	Non-uniform heat source/sink
σ^*	Stefan-Boltzmann constant
$k*$	Rosseland mean absorption coefficient

Physical Constants

Speed of Light	c	$=$	$2.997\ 924\ 58 \times 10^{8}\ \mathrm{ms}^{-1}$ (exact)
Acceleration due to gravity	g	$=$	$9.8\ \mathrm{ms}^{-2}$ (exact)
Stefan Boltzmann Constant	σ^{*}	$=$	$5.670\ 374\ 419 \times 10^{-8}\ \mathrm{Wm}^{-2}\ \mathrm{K}^{-4}$ (exact)

Chapter 1

Introduction

1.1 MHD Micropolar Fluids

The study of magnetic behaviour and properties of electrically conducting fluids is called Magnetohydrodynamics (MHD). The main idea behind MHD is that the magnetic fields induce currents in a moving conductive fluid, which in turn polarizes the fluid and in turn changes the magnetic field itself. The set of equations that can describe a MHD fluid behaviour are the combination of firstly the famous fluid dynamics equation i.e. the Navier–Stokes equations and Maxwell's equations of electromagnetism. This set of differential equations must be solved simultaneously, either analytically or numerically.

The simplest form of MHD, referred as the Ideal MHD assumes a fluid with so little resistivity so that it can be treated as a perfect conductor. This indeed is also the limit of infinite magnetic Reynolds number.

1.1.1 Ideal MHD Equations

The ideal MHD equations consist of:

1. Continuity equation
2. Cauchy momentum equation
3. Ampere's Law neglecting displacement current
4. Temperature evolution equation

The main quantities used to characterize electrically conducting fluid are the bulk plasma velocity field ν, the mass density ρ, the current density J, and the plasma pressure p. The flowing electric charge in the plasma then become the source of a magnetic field B along with an electric field E.

Mass continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$

Cauchy Momentum equation:

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = \mathbf{J} \times \mathbf{B} - \nabla p.$$

The Lorentz force term represented by J $\times$ B is then expanded using Ampere's law and the vector calculus identity

$$\tfrac{1}{2}\nabla(\mathbf{B} \cdot \mathbf{B}) = (\mathbf{B} \cdot \nabla)\mathbf{B} + \mathbf{B} \times (\nabla \times \mathbf{B})$$

to give

$$\mathbf{J} \times \mathbf{B} = \frac{(\mathbf{B} \cdot \nabla)\,\mathbf{B}}{\mu_0} - \nabla \left(\frac{B^2}{2\mu_0} \right),$$

where the first term and second term on the RHS represent magnetic tension force and the magnetic pressure force respectively.

Ideal Ohm's law for a plasma:

$$\mathbf{E} + \mathbf{v} \times \mathbf{B} = 0.$$

Faraday's law:

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}.$$

Low-frequency Ampère's law neglecting displacement current:

$$\mu_0 \mathbf{J} = \nabla \times \mathbf{B}.$$

Magnetic divergence constraint:

$$\nabla \cdot \mathbf{B} = 0.$$

Energy equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{p}{\rho^\gamma} \right) = 0,$$

where $\gamma = \frac{5}{3}$ is the adiabatic ratio of specific heats. This energy equation assumes that the entropy of a fluid element does not change and hence is only applicable in the absence of shocks or heat conduction.

1.2 Micropolar Fluids

Because of the increasing importance of material flow in industrial processing and elsewhere along with the fact that Newtonian relationships cannot characterize shear behavior, a new stage that accounts for this behaviour in the evaluation of fluid theory is in the progress. Eringen is infact attributed for the theory of molecular fluids which takes into account the inertial as well as rotational characteristics of the substructure particles. Physically, micropolar fluids have a suspension of small cylindrical elements such as large dumbbell-shaped molecules. The Micropolar theory has been generating an increased interest which has led to many classical flows being re-examined to determine the effects of the fluid microstructure.

As introduced earlier, Micropolar fluids deal with a class of fluids that exhibit microscopic effects arising from the micro-motions (such as micro-rotation and inertia) of the fluid elements. Micropolar fluids are those which contain micro-constituents that can undergo rotation which is a characteristic which was discarded in earlier researches. The presence of such characteristic can affect the hydrodynamics of the flow so that it is distinctly non-Newtonian. These fluids contain dilute suspension of rigid macro molecules with individual motions that support stress and body moments and are influenced by spin inertia.

In this work, the focus is on following problems: the first is to examine the influence that an external magnetic field along with a non-uniform heat source or sink and thermal radiation can have on the heat transfer and micropolar fluid flow over a stretching permeable surface. The second objective then is to implement and verify the novel numerical solution given by M.M. Khader using the fourth order predictor-corrector method for this physical problem. Further the use of suitable zero-finding algorithms uses the research done by P.D. Ariel and Serth in coming up with an effective trial function to contain the stream function of the particular problem.

Chapter 2

Problem Formulation

For the problem we consider in this research, consider an unsteady 2D mixed convection flow of an incompressible boundary layer flow of a MHD micropolar fluid over a permeable stretching sheet. Steady state is observed by the fluid for t $<$ 0 and at t $\geq$ 0, the fluid, heat along with mass flows are in unsteady state. We consider the stretching velocity of the permeable sheet as $u_w(x,t) = \frac{ax}{1-et}$. Furthermore, temperature and concentration of the sheet can be represented by $T_w(x,t) = T_\infty + \frac{bx}{1-et}$ and $C_w(x,t) = C_\infty + \frac{bx}{1-et}$, where a, b and e are some constants. As can be seen from Fig. 1, the stretching sheet velocity ($u_w(x,t)$) is taken along the x-axis and the Magnetic field of strength B is applied along y-direction which happen to be normal to the x-axis and under all the above mentioned assumptions, the governing equations of the flow can be demonstrated below:

Continuity Equation:

$\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} = 0$

Conservation of Momentum Equation:

$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \frac{\mu+k}{\rho}\frac{\partial^2 u}{\partial y^2} + \frac{k}{\rho}\frac{\partial N}{\partial y} + g\beta(T - T_\infty) + g\beta^*(C - C_\infty) - \sigma\frac{(\beta_0)^2}{\rho}u$

Conservation of Angular Momentum Equation:

$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} + v\frac{\partial N}{\partial y} = \frac{\gamma}{j\rho}\frac{\partial^2 N}{\partial y^2} - \frac{k}{j\rho}(2N + \frac{\partial u}{\partial y})$

Conservation of Energy Equation:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + u\frac{\partial T}{\partial y} = \frac{k}{\rho C_p}\frac{\partial q_r}{\partial y} + \frac{\mu+k}{\rho C_p}\frac{\partial u}{\partial y}^2 + \frac{\sigma\beta^2}{\rho C_p}u^2 + q^{'''}$$

Species Equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + y\frac{\partial C}{\partial y} = D_m\frac{\partial^2 C}{\partial y^2}$$

subject to the boundary conditions

$$u = \lambda U_m(x,t),\ v = v_w,\ N = -\frac{1}{2}\frac{\partial u}{\partial y},\ T = T_w(x,t),\ C = C_w(x,t),\ at\ y = 0$$
$$u \to 0,\ N \to 0,\ T \to T_\infty,\ C \to C_\infty,\ at\ y \to \infty$$

By introducing similarity variables followed by a few other manipulations we get the equivalent

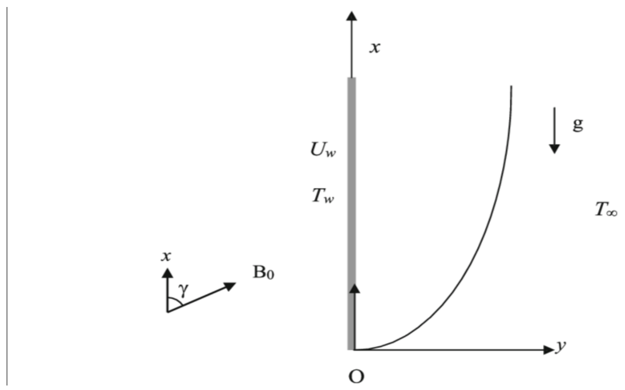

Figure 2.1: Coordinate system for the physical model

set of ODEs

$$(1+K)f^{'''} + ff^{''} - f^{'2} - \tau(f^{'} + \frac{1}{2}\xi f^{''}) + Kh^{'} + \delta\theta + \delta^*\phi - Mf^{''} = 0$$

$$(1+\frac{K}{2})h^{''} + \begin{vmatrix} f & f^{'} \\ h & h^{'} \end{vmatrix} - \tau(\frac{3}{2}h + \frac{1}{2}\xi h^{'}) - K(2h + f^{''}) = 0$$

$$(1+\frac{4}{3}R)\theta^{''} + Pr\begin{vmatrix} f & f^{'} \\ \theta & \theta^{'} \end{vmatrix} - Pr\cdot\tau(2\theta + \frac{1}{2}\xi\theta^{'}) + PrE_c(1+K)f^{''2} + PrME_cf^{'2} + A^*f^{'} + B^*\theta = 0$$

$$\phi'' + Sc \begin{vmatrix} f & f' \\ \phi & \phi' \end{vmatrix} - Sc \cdot \tau(\phi + \tfrac{1}{2}\xi\phi') = 0$$

Corresponding Boundary Conditions then become,

$f(0) = S,\ \ f'(0) = \lambda,\ \ h(0) = -\frac{1}{2}f''(0),\ \ \theta(0) = 1,\ \ \phi(0) = 1,$

$f'(\infty) = 0,\ \ h(\infty) = 0,\ \ \theta(\infty) = 0,\ \ \phi(\infty) = 0$

Chapter 3

Suggested Numerical Scheme of the Problem

3.0.1 PC4-FDM Method

For this particular problem, we apply the PC4-FDM method i.e. fourth order predictor-corrector method using finite difference method for obtaining the values of the 8 functions f, $f^{'}$ (Micropolar liquid velocity), h (Micro-rotation), $h^{'}$, θ (Temperature), θ, ϕ (Concentration) and $\phi^{'}$ at some particular points based to their values at the previous five mesh points.

3.0.1.1 Step-1 : (The Predictor-Step)

Using the following formulae for the derivative and double derivative operator in terms of the function value at the next mesh point and further approximating by a fourth-order approximation:
$D_{g\hbar} = \frac{1}{\hbar}(\nabla - \frac{1}{2}\nabla^2 - \frac{1}{3!}\nabla^3 - ...)g_{h+1}, \ \ D^2_{g\hbar} = \frac{1}{\hbar}(\nabla^2 - \frac{1}{2}\nabla^4 - \frac{1}{3!}\nabla^5 - ...)g_{h+1},$
where D is the derivative operator and ∇ is the backward operator, the above mentioned system can then be converted to the below mentioned system of algebraic equations in the form which can then be explicitly solved for $f_{i+1}, h_{i+1}, \theta_{i+1}, \phi_{i+1}, F_{i+1}, H_{i+1}, \Theta_{i+1} \ and \ \Phi_{i+1}$; i.e., by using the subscript s for the predicted values $(f^{(s)}, h^{(s)}, \theta^{(s)}, \phi^{(s)}, F^{(s)}, H^{(s)}, \Theta^{(s)}, \Phi^{(s)})$:

$$f^{(s)}_{i+1} = \frac{1}{3}\left(-10f_i + 18f_{i-1} - 6f_{i-2} + f_{i-3} + 12\hbar F_i\right)$$

$$h^{(s)}_{i+1} = \frac{1}{3}(-10h_i + 18h_{i-1} - 6h_{i-2} + h_{i-3} + 12\hbar H_i)$$

$\theta_{i+1}^{(s)} = \frac{1}{3}(-10\theta_i + 18\theta_{i-1} - 6\theta_{i-2} + \theta_{i-3} + 12\hbar\Theta_i)$

$\phi_{i+1}^{(s)} = \frac{1}{3}(-10\phi_i + 18\phi_{i-1} - 6\phi_{i-2} + \phi_{i-3} + 12\hbar\Phi_i)$

$F_{i+1}^{(s)} = (20(1+K) + 6\hbar f_i - 3\hbar\tau\xi_i)^{-1}\left[-\left(30(1+K) + 20f_i\hbar - 10\hbar\tau\xi_i - 24\hbar^2(\tau+M)\right)F_i + \right.$
$(8(1+K) + 36f_i\hbar - 18\hbar\tau\xi_i)F_{i-1} - (28(1+K) + 12f_i\hbar - 6\hbar\tau\xi_i)F_{i-2} +$
$\left.(12(1+K) + 2f_i\hbar - \hbar\tau\xi_i)F_{i-3} + 2(1+K)F_{i-4} + 24\hbar^2(F_i^2 - KH_i - \delta\theta_i - \delta^*\phi_i)\right]$

$H_{i+1}^{(s)} = \frac{1}{3}\left[-\left(10 + 12\hbar(1+0.5K)^{-1}(f_i - 0.5\tau\xi_i)\right)H_i + 18H_{i-1} - 6H_{i-2} + H_{i-3} + \right.$
$\left.(1+0.5K)^{-1}\left(K\left(3F_{i+1} + 10F_i - 18F_{i-1} + 6F_{i-2} - f_{i-3}\right) + 12\hbar\left(F_i + 1.5\tau + 2K\right)h_i\right)\right]$

$\Theta_{i+1}^{(s)} = \frac{1}{3\hbar}\left[-\left(10\hbar + 12\hbar^2(1+\frac{4}{3}R)^{-1}Pr(f_i - 0.5\tau\xi_i)\right)\Theta_i + 18\hbar\Theta_{i-1} - 6\hbar\Theta_{i-2} + \hbar\Theta_{i-3} - \right.$
$12PrEc(1+K)(1+\frac{4}{3}R)^{-1}\left(\frac{1}{4}F_{i+1} + \frac{5}{6}F_i - \frac{3}{2}F_{i-1} + \frac{1}{2}F_{i-2} - \frac{1}{12}F_{i-3}\right)^2 +$
$\left.12\hbar^2(1+\frac{4}{3})^{-1}\left(Pr\theta_i(F_i+\tau) - PrMEcF_i^2 - A^*F_i - B^*\theta_i\right)\right]$

$\Phi_{i+1}^{(s)} = \frac{1}{3}\left[-\left(10 - 6\hbar\tau Sc\xi_i + 12\hbar Scf_i\right)\Phi_i + 18\Phi_{i-1} - 6\Phi_{i-2} + \Phi_{i-3} + 12\hbar\phi Sc(\tau + F_i)\right]$

3.0.1.2 Step-2 : (The Corrector-Step)

Using the following operators i.e the derivative and double derivative operator in terms of the value of the function at the current mesh point and by again applying a fourth-order approximation
$D_{g\hbar} = \frac{1}{\hbar}(\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + ...)g_h,\ \ D_{g\hbar}^2 = \frac{1}{\hbar}(\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \frac{5}{6}\nabla^5 + ...)g_h,$
we obtain the corrected values for the 8 functions which were defined above:
$f_{i+1} = \frac{1}{25}\left(48f_i - 36f_{i-1} + 16f_{i-2} - 3f_{i-3} + 12\hbar F_{i+1}^{(s)}\right)$

$h_{i+1} = \frac{1}{25}\left(48h_i - 36h_{i-1} + 16h_{i-2} - 3h_{i-3} + 12\hbar H_{i+1}^{(s)}\right)$

$\theta_{i+1} = \frac{1}{25}\left(48\theta_i - 36\theta_{i-1} + 16\theta_{i-2} - 3\theta_{i-3} + 12\hbar\Theta_{i+1}^{(s)}\right)$

$\phi_{i+1} = \frac{1}{25}\left(48\phi_i - 36\phi_{i-1} + 16\phi_{i-2} - 3\phi_{i-3} + 12\hbar\Phi_{i+1}^{(s)}\right)$

$F_{i+1} = (20(1+K) + 50\hbar f_i - \hbar\tau\xi_i)^{-1}\left[-\left(30(1+K) - 96f_i\hbar - 48\hbar\tau\xi_i - 24\hbar^2(\tau+M)\right)F_i + \right.$
$(8(1+K) - 72f_i\hbar + 36\hbar\tau\xi_i)F_{i-1} - (28(1+K) - 32f_i\hbar + 16\hbar\tau\xi_i)F_{i-2} + (12(1+K) - 6f_i\hbar + 3\hbar\tau\xi_i)F_{i-3} +$

$2(1+K)F_{i-4}+24\hbar^2(F_i^2-KH_i-\delta\theta_i-\delta^*\phi_i)]$

$H_{i+1}=\frac{1}{25}[\left(48-12\hbar(1+0.5K)^{-1}(f_i-0.5\tau\xi_i)\right)H_i-36H_{i-1}+16H_{i-2}-3H_{i-3}+(1+0.5K)^{-1}$
$(K\,(25F_{i+1}-48F_i+36F_{i-1}-16F_{i-2}+3F_{i-3})+12\hbar\,(F_i+1.5\tau+2K)\,h_i)]$

$\Theta_{i+1}=\frac{1}{25\hbar}[\left(48\hbar-12\hbar^2(1+\frac{4}{3}R)^{-1}Pr(f_i-0.5\tau\xi_i)\right)\Theta_i-36\hbar\Theta_{i-1}+16\hbar\Theta_{i-2}-3\hbar\Theta_{i-3}-$
$12PrEc(1+K)(1+\frac{4}{3}R)^{-1}\left(\frac{25}{12}F_{i+1}-4F_i+3F_{i-1}-\frac{4}{3}F_{i-2}-\frac{1}{4}F_{i-3}\right)^2+12\hbar^2(1+\frac{4}{3})^{-1}$
$\left(Pr\theta_i(F_i+\tau)-PrMEcF_i^2-A^*F_i-B^*\theta_i\right)]$

$\Phi_{i+1}=\frac{1}{25}\left[(48+12\hbar\tau Sc\xi_i-12\hbar Scf_i)\,\Phi_i-36\Phi_{i-1}+16\Phi_{i-2}-3\Phi_{i-3}+12\hbar\phi Sc(\tau+F_i)\right]$

From the above derived system of couple ODEs along with their boundary conditions we can see that the values of $f, f^{'}, h, \theta$ and ϕ are given at 0 (Lower boundary point of [0,η_∞]), but the values of f, h, θ and ϕ are given at ∞(Upper boundary point of [0,η_∞]), the proposed system is a Boundary Value Problem (BVP). Therefore, to convert this BVP to an Initial Value Problem (IVP) we change the initial guess of $f^{''}, h^{'}, \theta^{'}$ and $\phi^{'}$ so that the boundary conditions at ∞ are satisfied. Let us start with an initial guess for the value of $f^{''}, h^{'}, \theta^{'}$ and $\phi^{'}$ at zero which can be defined as follows:

$f^{''}(0)=l_1,\ h^{'}(0)=l_2,\ \theta^{'}(0)=l_3,\ \phi^{'}(0)=l_4$

As can be seen from the above equations for the PC4-FDM method, we need values of the 8 functions $f, h, \theta, \phi, F, H, \Theta$, and Φ at previous five mesh points to get the value at the current mesh point. Hence to start the solution, we need to first find the values of these functions at $\xi=\pm h\xi=\pm 2h\xi$ by applying the Taylor series. Around $\xi=0$, taylor series for expansion of f, h, θ and ϕ takes the following form:

$f(\xi)=\sum_{j=0}^{5}a_j\xi^j,\ h(\xi)=\sum_{j=0}^{5}b_j\xi^j,\ \theta(\xi)=\sum_{j=0}^{5}c_j\xi^j,\ \phi(\xi)=\sum_{j=0}^{5}d_j\xi^j,$

where a_j, b_j, c_j and d_j are constants whose values can be obtained by using the boundary conditions of the 8 functions mentioned above$f, h, \theta, \phi, F, H, \Theta$, and Φ. Henceforth, 9 of the above mentioned constants $a_0, a_1, a_2, b_0, b_1, c_0, c_1, d_0$ and d_1 are obtained on the basis of boundary values of these functions at $\xi=0$ and others are obtained by replacing the functions with their taylor series expansion in the above set of coupled ODEs.

$a_0 = S,\ a_1 = \lambda,\ b_0 = -\frac{l_1}{2},\ c_0 = 1,\ c_1 = 1,$

$a_2 = \frac{l_1}{2},\ b_1 = l_2,\ c_1 = l_3,\ d_1 = l_4$

The remaining constants which are to be obtained from the set of ODE can be done by substituting values of functions obtained at $\xi = 0$ and by using the Taylor series expansion.

$a_3 = (M\lambda - \delta^* - \delta - Kl_2 + \tau\lambda + \lambda^2 - Sl_1)(6(1+K))^{-1}$

$b_2 = (2Ka_2 + 2Kb_0 + \frac{3\tau b_0}{2} + b_0a_1 - a_0b_1)(2(1+\frac{K}{2}))^{-1}$

$a_4 = (2Ma_2 - \delta^* d_1 - \delta c_1 - 2Kb_2 + 3\tau a_2 + 2a_1a_2 - 6a_0a_3)(24(1+K))^{-1}$

$b_3 = (6Ka_3 + 2Kb_1 + 2\tau b_1 + 2a_2b_0 - 2a_0b_2)(6(1+\frac{K}{2}))^{-1}$

$c_2 = (2Pr\tau c_0 - Pr(a_0c_1 - a_1c_0) - 4PrEc(1+K)a_2^2 - PrMEca_1^2 - A^*a_1 - B^*c_0)(2*(1+\frac{4R}{3}))^{-1}$

$c_3 = (\frac{5\tau Prc_1}{2} - 24PrEc(1+K)a_2a_3 - 4PrEcMa_1a_2 - 2A^*a_2 - B^*c_1 - 2Pr(a_0c_2 - a_2c_0))(6(1+\frac{4R}{3})^{-1}$

$c_4 = (6Pr\tau c_2 - 2PrEc(1+K)(48a_2a_4 + 36a_3^2) - Pr(6a_0c_3 - 6a_3c_0) - 4PrMEc(2a_2^2 + 3a_1a_2) - 6A^*a_3 - 2B^*c_2)(24(1+\frac{4R}{3}))^{-1}$

$d_2 = (Sc\tau d_0 - Sc(a_0d_1 - d_0a_1))/2$

$a_5 = (6Ma_3 - 2(\delta c_2 + \delta^* d_2) - 6Kb_3 + 12a_3\tau + 4a_2^2 - 24a_0a_4)(60(1+K))^{-1}$

$c_5 = (21Pr_3 - Pr(12a_1c_3 - 12a_3c_1 + 24c_0c_4 - 24a_4c_0) - 2PrEc(1+K)(120a_2a_5 + 432a_3a_4) - 2PrMEc(36a_2a_3 + 24a_1a_4) - 24A^*a_4 - 6B^*c_3)(60(1+\frac{4R}{3}))^{-1}$

$d_3 = (\frac{3Sc\tau d_1}{2} - 2Sc(a_0d_2 - d_0a_2))/6$

$d_4 = (4Sc\tau d_2 - Sc(12a_1d_3 - 12d_1a_3 + 24a_0d_4 - 24d_0a_4))/60$

$b_4 = (K(4b_2 + 24a_4) + 5\tau b_2 + 6a_3b_0 + 2a_2b_1 - 6a_0b_3 - 2a_1b_2)(24(1+\frac{K}{2}))^{-1}$

$b_5 = (K(12b_3 + 60a_5) + 18b_3\tau + 24a_4b_0 - 24a_0b_4 + 12a_3b_1 - 12a_1b_3)(60(1+\frac{K}{2}))^{-1}$

Now, that we have the values for all the constants a_j, b_j, c_j and d_j, one can get the Taylor series expansion for f, h, θ and ϕ around $\xi = 0$. These equations can hence be used to find the value of these four functions at the initial 5 mesh points which are needed to start the PC4-FDM Method for finding the solution to the set of ODEs.

The implementation of the above mentioned algorithm for the fourth-order predictor-corrector method can now be summarized:

(i) Firstly, values are assigned to ξ_∞, which is taken as the upper boundary condition for the solution space, basically an approximation to infinity; $\hbar$, the step-size for applying finite difference method to the solution space and other constants such as the Magnetic field parameter, heat source/sink parameters, etc.

(ii) Secondly, to start the solution suggested an intial guess is made for $l_1(= f"(0)), l_2(= h'(0)), l_3(= \theta'(0))$ and $l_4(= \phi'(0))$.

(iii) Next, using the Taylor series expansion mentioned above, values of the functions f, h, θ and ϕ are computed at $\xi = \pm\hbar$ and $= \pm 2\hbar$.

(iv) Lastly, the predictor-corrector method defined is then applied repeatedly to advance the values of the 8 functions f, f', h, h', θ, θ', ϕ and ϕ' by one integration step ($\hbar$) until values for all these functions are computed at all mesh-points of the solution space.

(v) After completion of the method, we then check if the values of f"(0), h'(0), $\theta'(0)$ and $\phi'(0)$ agrees to 0 within the prescribed accuracy or not. The results are accepted if the same happens, else new values of l_1, l_2, l_3 and l_4 need to be calculated and then the steps (iii)-(v) are again repeated till we obtain the desired results.

3.0.2 Gear's Method

Piggybacking on Gear's Method:

Given the quantity of constants that needed to be perfected in this particular problem, the approach was to piggyback on the implementation of a previous research on the same method i.e. Fourth order predictor-corrector method but with fewer equations and constants. The first research that simplified the method was by M.M. Khader in "Fourth-order predictor-corrector FDM for the effect of viscous dissipation and Joule heating on the Newtonian fluid flow". The second research that further simplified the method was by P.D. Ariel in "Generalized Gear's method for computing the flow of a viscoelastic fluid".

3.0.2.1 2D stagnation point flow

This section introduces the most extensively studied and investigated problem among all flow problems of viscoelastic problems i.e. the 2D stagnation point flow of a viscoelastic fluid.

$f''' + ff'' + 1 - f'^2 + k(ff^{iv} - 2f'f''' + f''^2) = 0,$

$f(0) = 0, f'(0) = 0, f'(\infty) = 1,$

where f represents the dimensionless stream function, k is the viscoelastic fluid parameter and a prime after the function denotes the derivative of that function with respect to η, the similarity variable.

After applying all the steps mentioned above for the fourth-order predictor-corrector method, we are able to compute the equations for f, f' and f" which can be used to generate the values of these functions for any solution space. From the boundary condition specified in the problem we can see that the values of f and f' are given at n = 0 but since f' is given at infinity, above problem can be thought of as a BVP. To convert this to an IVP we used the similar aforementioned method i.e. make an guess for the missing initial condition, namely, the value of f"(0). Hence, let $f"(0) = s$.

The quantity s is be chosen such that the terminal condition is satisfied. Therefore, assuming that s is known, we get all the initial conditions at $\eta = 0$. As a next step and in order to start the solution method, we need the values at four more points, which we choose $\eta = \pm h = \pm 2h$ as in the previous problem of unsteady micropolar fluid flow. To obtain these values again we take help from the Taylor series expansion for $f(\eta)$ around $\eta = 0$:

$f = \sum_{i=0}^{5} c_i \eta^i$

where $c_i s$ are constants. From the initial boundary conditions, the first three $c_i s$ are calculated:

$c_0 = 0,\ c_1 = 0,\ c_2 = \frac{1}{2}s$

The remaining constants are further obtained by substituting the Taylor series expression mentioned above in the equation for 2D stagnation point flow.

$c_3 = -\frac{Ks^2+1}{6},\ c_4 = 0,\ c_5 = \frac{s^2}{120}$

Now once the steps (i)-(iv) are completed the next problem that needs to be addressed is one of selecting a suitable zero finding algorithm to effectively compute the initial value for f". Recently, researches around the world have tried to employ several weighted residual methods (MWR) to obtain solutions to the laminar boundary layer equations. The reason behind the sudden increase of interest in researchers world wide can be attributed to the accuracy of such methods which is in a very close range to the solutions obtained from the method of finite difference. Furthermore these methods require considerably less computing time. We shall examine one such method i.e. of orthogonal collocation which is then employed to find the solution for 2D stagnation point flow problem.

3.0.2.2 Serth's Method - Orthogonal Collocation

The method of orthogonal collocation firstly requires the selection of an orthogonal basis for $L^2(0, \infty)$, which is the Hilbert space of Lebesgue square-integrable functions on $(0, \infty)$. The first choice for the same can be that involving set of Laguerre functions and for that case, an appropriate trial function for $f(\eta)$ becomes

$f(\eta) = -1 + \eta + e^{-\eta} + \eta^2 \sum_{k=1}^{N} C_k \psi_{k-1}(\eta)$

Here, the $\psi_k(\eta)$ are the Laguerre functions,

$\psi_k(\eta) = e^{-\eta/2} L_k(\eta)$

and $L_k(\eta)$ is the Laguerre polynomial of degree k. The constants $C_1, C_2, ..., C_N$ can be determined by the process of collocation at the N zeros of $L_k(\eta)$.

An alternative basis for$L^2(0, \infty)$ is the set of orthogonal exponential functions. In this case it is convenient to first apply the transformation

$\xi = e^{\eta}, F(\xi) = f(\eta)$

The function $F(\xi)$ then satisfies the boundary conditions

$F(1) = F'(1) = 0, \lim_{\xi \to 0} \xi F'(\xi) = -1$

All this leads to an appropriate trial function:

$F(\xi) = \xi - 1 - ln\xi + (\xi - 1)^2 \sum_{k=1}^{N} C_k P_{k-1}(\xi)$

where $P_k(\xi)$ is a set of orthogonal polynomials on (0, 1).

Serth studies 3 sets of orthogonal polynomials namely the shifted Legendre polynomials and the shifted Chebyshev polynomials of the first and second kind. In this implementation however, only shifted Legendre polynomials have been considered. The constants C_k in the above trial function are again evaluated by collocation at the N zeros of the shifted Legendre polynomials. The problem is then reduced to the solution of N simultaneous nonlinear equations. The solution in Serth's was then obtained by means of Marquardt's method i.e. "An algorithm for least squares estimation of nonlinear parameters." In this case however, inbuilt MATLAB function has been used for the same.

Chapter 4

Results and Discussion

4.0.1 2D Stagnantion Point Flow

The program was initially run for values of k=0, 0.1, 0.2 and 0.3. In Figure 4.1, f is plotted against η for the above values of k. The graph can then be compared with the results obtained by P.D. Ariel which are shown in Figure 4.2 and 4.4.

For the same values of k, f' is plotted against q in Figure 4.3. The most interesting feature of

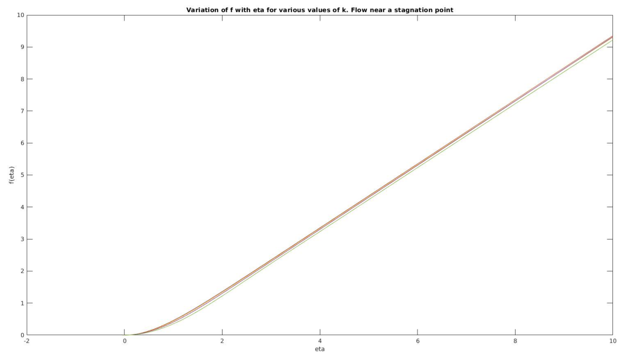

FIGURE 4.1: Variation of f with η

these results is that the velocity in the boundary layer oscillates about its value in the mainstream for sufficiently large values of q when $k \neq 0$, i.e. for the viscoelastic fluids, though the oscillations damp out with increasing q. This phenomenon is more pronounced for higher values of k (e.g. k = 0.3), but it was also observed for low values of k (k=0.05). A similar observation was also reported by Teipel for the flow of a second-order fluid near a stagnation point. These results thus vindicate the conclusions of Beard and Walters.

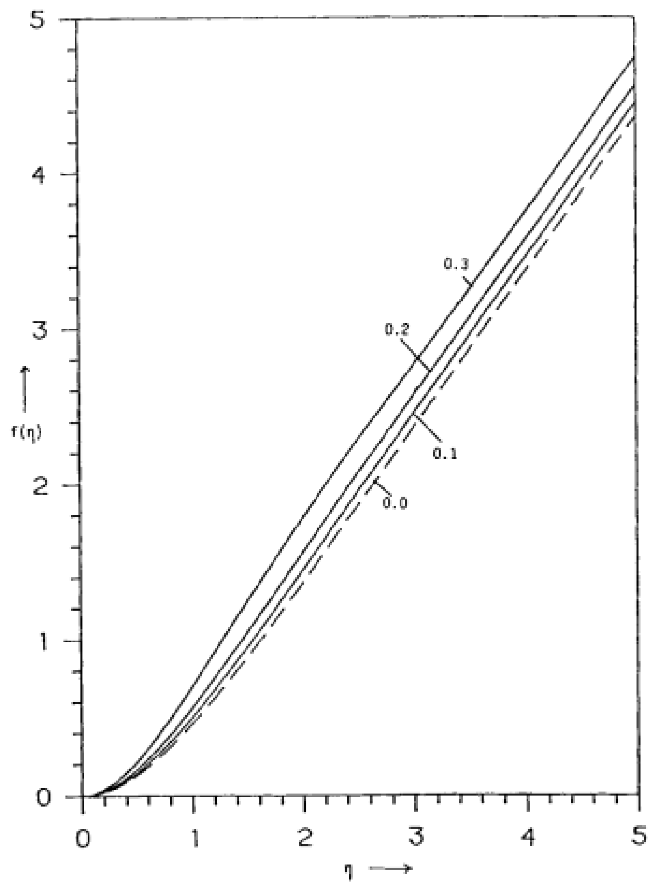

FIGURE 4.2: Variation of f with η - P.D. Ariel

The results of the solution of the 2D stagnation-point flow with the proposed fourth-order

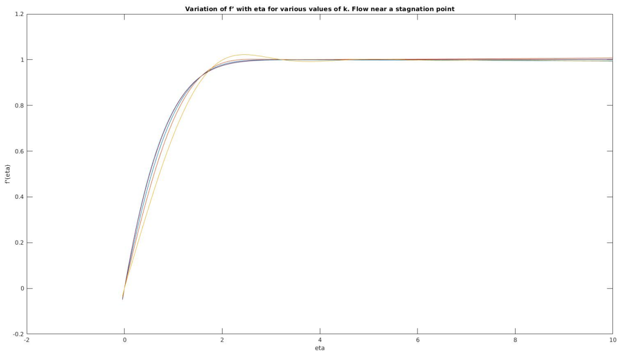

FIGURE 4.3: Variation of f' with η

predictor-corrector method are presented in Table 1.

From the values mentioned in Table 1, it can be easily concluded that the step size h must be smaller than 0.05 to obtain reliable values of the initial value of f" i.e. f"(0) which is the key

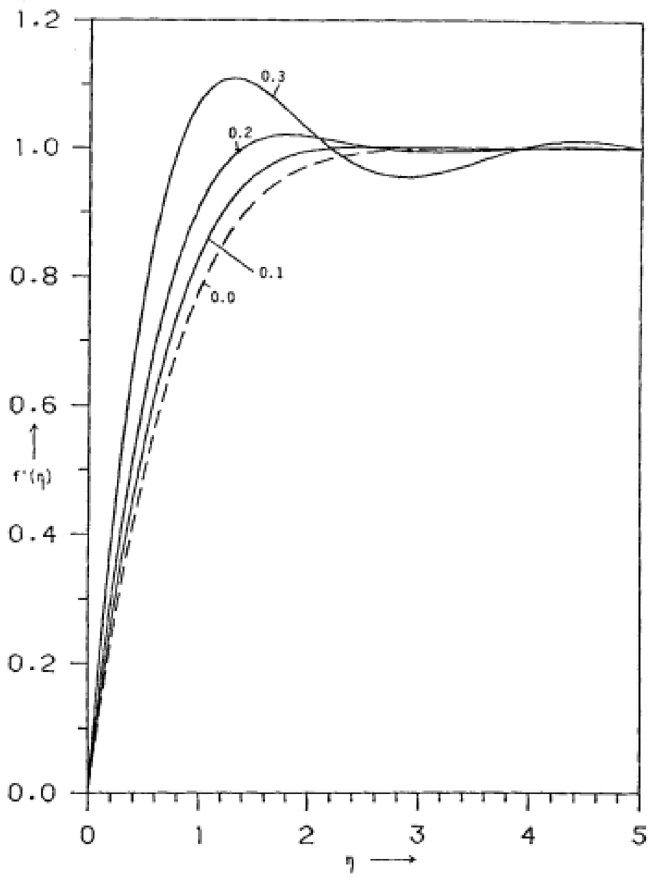

FIGURE 4.4: Variation of f' with η - P.D. Ariel

K (Weissenberg Number)	h=0.1	h=0.05	h=0.02	h=0.01	Serth	Present Study
0	1.201388826	1.21349757	1.213566436	—	1.232587	1.23258
0.05	1.294618079	1.29464226	1.294646606	1.294646	1.294646	1.1067
0.1	1.369500992	1.36953449	1.369541015	1.369539	1.369538	0.9939
0.2	1.560314529	1.58732493	1.587328125	1.587328	1.587332	0.8171
0.3	1.088899532	1.13850445	2.110821533	2.110818	—	0.6977

TABLE 4.1: Variation of s=f"(0) with variation in viscoelastic parameter in 2-D stagnation-point flow

point in the solution method proposed for the above problem of 2D stagnation point flow. The sheer parameter at solid boundary in a particular location of the domain depends linearly on f"(0). So, from the above table it can be understood that for larger values of f"(0), shear stress on the solid boundary is larger as compared to those with smaller values of f"(0). Therefore, it can be concluded from Table 1 that this parameter decreases as Weissenberg number (Viscoelastic parameter) increases.

4.0.2 Unsteady MHD Micropolar Fluid Flow

For the case of $M = R = E_c = K = A = B = \delta = 0$ and $Pr = 1$,

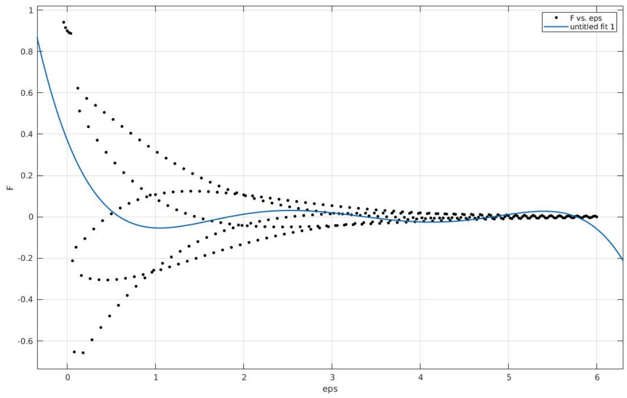

FIGURE 4.5: Micro-polar fluid velocity

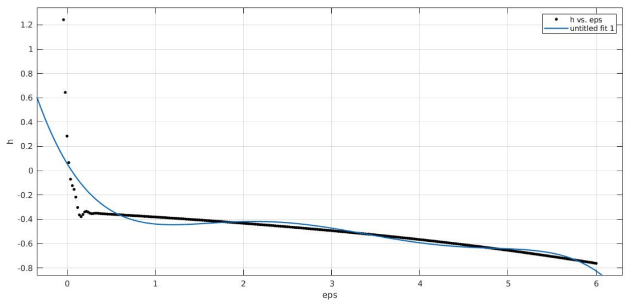

FIGURE 4.6: Micro-polar fluid angular momentum

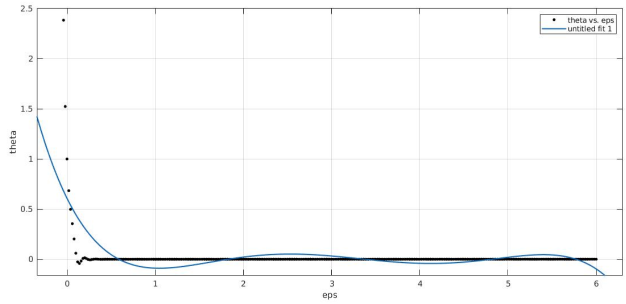

FIGURE 4.7: Micro-polar fluid Temperature

Coming to the results for the Research carried out by M.M. Khader for an unsteady, incompressible MHD micropolar fluid flow with thermal radiation and heat source past a stretching sheet.

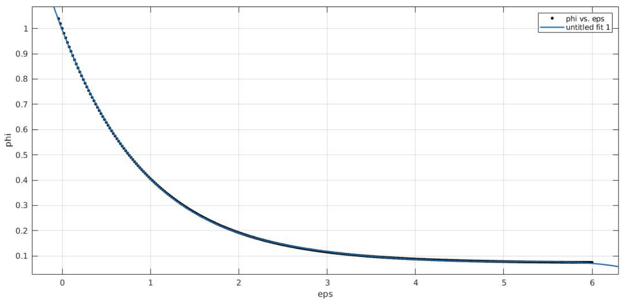

FIGURE 4.8: Micro-polar fluid Concentration

The proposed method for this particular problem i.e. the Fourth order predictor–corrector FDM method has been successfully implemented and verified to solve the problem. The results presented graphically indicate the variation of the 4 functions (Micro-polar fluid velocity, fluid angular momentum, temperature and concentration) with respect to various system parameters (such as Prandtl number, Micropolar fluid temperature, etc). From the graphical results obtained, the following conclusions can be deduced:

- A positive correlation is observed between the Prandtl number and the velocity and temperature profiles whereas an reverse trend i.e. a negative correlation is seen for the angular momentum and concentration profiles;
- Concentration, Micropolar fluid temperature and angular momentum profiles indicate a positive correlation with respect to the value of magnetic parameter while a reverse trend or negative correlation is observed for velocity profile;
- Temperature and Micropolar fluid velocity profiles indicate a positive correlation with respect to the values of the thermal radiation parameter while a negative correlation can be concluded for the angular momentum and concentration profiles;
- Temperature, Micropolar liquid velocity and angular momentum profiles enhance with the increase in the values of micropolar parameter whereas the values of concentration profile diminish hence suggest a negative correlation;
- Micropolar liquid velocity, temperature, angular momentum as well as concentration profiles exhibit a negative correlation with respect to the unsteadiness parameter;

- Micropolar liquid velocity profile show a reduction in its values for rising values of the concentration buoyancy parameter indicating a negative correlation unlike that for the temperature, angular momentum and concentration profiles;
- The Micropolar fluid velocity and temperature profiles show an enhancement with the increased values of the Eckert number suggesting a positive correlation unlike while that for the angular momentum and concentration profiles;
- Micropolar fluid velocity and temperature profiles show an enhancement with the increased values of the temperature dependent internal heat source/sink parameter unlike that for angular momentum and concentration profiles;

Appendix A

MATLAB Code-Gear's Method

```
%% Generalize Gear's method for computing the flow of a viscoelastic fluid %%
%% Author: P. Donald Ariel %%

ninf=10;                                                %% n_infinity
h=0.02;                                                 %% step size
n=(ninf)/h+3;                                           %% number of iterations
eta=-2*h:h:ninf;                                        %% Mesh Points
k=[0 0.01 0.05 0.1 0.2 0.3];                    %% viscoelastic fluid parameter
s=[1.232587 1.2069 1.1067 0.9939 0.8171 0.6977];        %% f''(0)=Q(0)=s
c(1)=0;                                                 %% Constant c0
c(2)=0;                                                 %% Constant c1
epsilon=10^(-3);                                        %% error tolerance
err=1;                                                  %% current error
Z=zeros(4,n);
for y=1:5
    while err>epsilon
        f=zeros(1,n);            %% function f
        fp=zeros(1,n);           %% function fp (predicted value of f)
        P=zeros(1,n);            %% function f'=P
        Pp=zeros(1,n);           %% function fp (predicted value of P)
        Q=zeros(1,n);            %% function f''=Q
        Qp=zeros(1,n);           %% function fp (predicted value of Q)
```

```
    c(3)=s(y)/2;                        %% constant c2
    c(4)=-1*(1+4*k(y)*(c(3)^2))/6;      %% constant c3
    c(5)=0;                             %% constant c4
    c(6)=(c(3)^2)/30;                   %% constant c5

    %%%%----------Function values at first 5 mesh points------------%%%

    for i=1:5
        for j=1:6
                f(i)=f(i)+c(j)*(((i-3)*h)^(j-1));
        end
    end
    for i=1:5
        for j=1:5
            P(i)=P(i)+j*c(j+1)*(((i-3)*h)^(j-1));
        end
    end
    for i=1:5
        for j=1:4
            Q(i)=Q(i)+j*(j+1)*c(j+2)*(((i-3)*h)^(j-1));
        end
    end

    %%%%------------Fourth-order Predictor-Corrector----------------%%%

    for i=5:n-1
        fp(i+1)=(-10*f(i)+18*f(i-1)-6*f(i-2)+f(i-3)+12*h*P(i))/3;
        Pp(i+1)=(-10*P(i)+18*P(i-1)-6*P(i-2)+P(i-3)+12*h*Q(i))/3;
        Qp(i+1)=(k(y)*f(i)*(15*Q(i)+4*Q(i-1)-14*Q(i-2)+6*Q(i-3)-
        Q(i-4))+h*(1-2*k(y)*P(i))*(-10*Q(i)+18*Q(i-1)-6*Q(i-2)+Q(i-3))-
        12*(h^2)*(f(i)*Q(i)+1-(P(i)^2)+k(y)*(Q(i)^2)))/(10*k(y)*f(i)+
        3*h*(1-2*k(y)*P(i)));
        f(i+1)=(48*f(i)-36*f(i-1)+16*f(i-2)-3*f(i-3)+12*h*Pp(i+1))/25;
        P(i+1)=(48*P(i)-36*P(i-1)+16*P(i-2)-3*P(i-3)+12*h*Qp(i+1))/25;
```

```
            Q(i+1)=(k(y)*fp(i+1)*(154*Q(i)-214*Q(i-1)+156*Q(i-2)-61*Q(i-3)+
            10*Q(i-4))+h*(1-2*k(y)*Pp(i-1))*(48*Q(i)-36*Q(i-1)+16*Q(i-2)-
            3*Q(i-3))-12*(h^2)*(fp(i+1)*Qp(i+1)+1-(Pp(i+1)^2)+
            k(y)*(Qp(i+1)^2)))/(45*k(y)*fp(i+1)+25*h*(1-2*k(y)*Pp(i+1)));
        end

        %%%%------Orthogonal collocation using Legendre Polynomial------%%%

        D=optimvar('D',4);  %% Lengendre Constants C
        xi=exp(-1*eta);  %% From serth's paper the transform from eta to xi
        %syms f(xi);
        fun=xi-1-log(xi)+power(xi-1,2).*(D(1)+D(2)*(2.*xi-1)+D(3)*(6*power(xi,2)
        -6.*xi+1)+D(4)*(20*power(xi,3)-30*power(xi,2)+12.*xi-1));
        %fun=-xi.*(1-(1./xi)+2*(xi-1).*(D(1)+D(2)*(2.*xi-1)+D(3)*(6*power(xi,2)
        %-6.*xi+1)+D(4)*(20*power(xi,3)-30*power(xi,2)+12.*xi-1))+
        %power(xi-1,2).*(2*D(2)+D(3)*(12.*xi-6)+D(4)*(60*power(xi,2)-60.*xi+12))
        obj=sum((fun-f).^2);    %% Objective function
        lsqproblem=optimproblem("Objective",obj);
        x0.D=[3/2 1/2 3/2 1/2];
        [sol,fval] = solve(lsqproblem,x0);
        responsedata = evaluate(fun,sol);
        show(lsqproblem)
        fns = fieldnames(sol);
        %A.(fns{3})
        g=sol.(fns{1});
        s(y)=(1+2*(g(1)+g(2)+g(3)+g(4))); %% Updated value of the constant
        %g=diff(diff(responsedata));
        %plot(g);
        %s=g;
        err=evaluate(obj,sol);
        x=evaluate(fun,sol);                    %% Updated error
        %figure(1)
        %plot(x)
        %hold on
```

```
        %plot(f)
        %plot(P,f,'r*',f,responsedata,'b-')
        %legend('Original Data','Fitted Curve')
        %xlabel 't'
        %ylabel 'Response'
        %title("Fitted Response")%%
    end
    Z(y,:)=f;
end
figure(1)
for y=1:5
    plot(eta,Z(y,:));
    hold on;
end
title("Variation of f with eta for various values of k") ;
xlabel("eta") ;
ylabel("f(eta)") ;
%figure(2)
%plot(eta,f);
%figure(3)
%plot(eta,P);
%figure(4)
%plot(eta,Q);
```

Appendix B

MATLAB Code-Unsteady MHD Micropolar fluid flow

```
%% Evaluating the unsteady MHD micropolar fluid flow past
%% stretching/shirking sheet with heat source and thermal radiation:
%% Implementing fourth order predictor{corrector FDM
%% Author: M.M. Khader and R.P. Sharma %%

%%%---------------------------Basic Constants---------------------------%%%

Sc=0.04;                    %% Schmidt number
tau=2;                      %% unsteadiness parameter
delta=0;                    %% Thermal Buoyancy parameter
M=0;                        %% Concentration buoyancy parameter
R=0;                        %% Thermal radiation parameter
Ec=0;                       %% Eckart Number
K=0;                        %% Micropolar parameter
A1=0;                       %% A*
B1=0;                       %% B*
delta1=0;                   %% delta*
Pr=1.0;                     %% Prandtl Number
xinf=6;                     %% n_infinity
hstep=0.02;                 %% step size
```

```
N=(xinf)/hstep+3;           %% number of iterations
eps=-2*hstep:hstep:xinf;    %% Mesh Points
S=25;                       %% Suction/injection paramter
lambda=0.9;                 %% stretching/shrinking parameter
l1=zeros(1,N);              %% f''(0)=l1
l2=zeros(1,N);              %% h'(0)=l2
l3=zeros(1,N);              %% theta'(0)=l3
l4=zeros(1,N);              %% phi'(0)=l4

%%%---------------------------Initial Constants--------------------------%%%

l1(1)=-0.8;
l2(1)=-1;
l3(1)=-1;
l4(1)=-0.95;
%l1(2)=-1.1;
epsilon=10^(-5);
err=1;                  %error for the values of l1(k), l2(k), l3(k) and l4(k)
k=1;
%%%-----------------Equations for constant determining------------------%%%
while err>epsilon && k<4
    a(1)=S;                         %% a0
    a(2)=lambda;                    %% a1
    a(3)=l1(k)/2;                   %% a2
    b(1)=-1*l1(k)/2;                %% b0
    b(2)=l2(k);                     %% b1
    c(1)=1;                         %% c0
    c(2)=l3(k);                     %% c1
    d(1)=1;                         %% d0
    d(2)=l4(k);                     %% d1
    a(4)=(M*lambda-delta1-delta-K*l2(k)+tau*lambda+lambda^2-S*l1(k))/(6*(1+K));
    b(3)=(2*K*a(3)+2*K*b(1)+3*tau*b(1)/2+b(1)*a(2)-a(1)*b(2))/(2*(1+K/2));
    a(5)=(2*M*a(3)-delta1*d(2)-delta*c(2)-2*K*b(3)+3*tau*a(3)+2*a(2)*a(3)-
    6*a(1)*a(4))/(24*(1+K));
```

```
b(4)=(6*K*a(4)+2*K*b(2)+2*tau*b(2)+2*a(3)*b(1)-2*a(1)*b(3))/(6*(1+K/2));
c(3)=(2*Pr*tau*c(1)-Pr*(a(1)*c(2)-a(2)*c(1))-4*Pr*Ec*(1+K)*a(3)*a(3)-
Pr*M*Ec*a(2)*a(2)-A1*a(2)-B1*c(1))/(2*(1+4*R/3));
c(4)=(5*tau*Pr*c(2)/2-24*Pr*Ec*(1+K)*a(3)*a(4)-4*Pr*Ec*M*a(2)*a(3)-
2*A1*a(3)-B1*c(2)-2*Pr*(a(1)*c(3)-a(3)*c(1)))/(6*(1+4*R/3));
c(5)=(6*Pr*tau*c(3)-2*Pr*Ec*(1+K)*(48*a(3)*a(5)+36*a(4)*a(4))-
Pr*(6*a(1)*c(4)-6*a(4)*c(1))-4*Pr*M*Ec*(2*a(3)*a(3)+3*a(2)*a(3))-6*A1*a(4)-
2*B1*c(3))/(24*(1+4*R/3));
d(3)=(Sc*tau*d(1)-Sc*(a(1)*d(2)-d(1)*a(2)))/2;
a(6)=(6*M*a(4)-2*(delta*c(3)+delta1*d(3))-6*K*b(4)+12*a(4)*tau+4*a(3)*a(3)
-24*a(1)*a(5))/(60*(1+K));
c(6)=(21*Pr*tau*c(4)-Pr*(12*a(2)*c(4)-12*a(4)*c(2)+24*c(1)*c(5)-
24*a(5)*c(1))-2*Pr*Ec*(1+K)*(120*a(3)*a(6)+432*a(4)*a(5))-
2*Pr*M*Ec*(36*a(3)*a(4)+24*a(2)*a(5))-24*A1*a(5)-6*B1*c(4))/(60*(1+4*R/3));
d(4)=(3*Sc*tau*d(2)/2-2*Sc*(a(1)*d(3)-d(1)*a(3)))/6;
d(5)=(4*Sc*tau*d(3)-Sc*(2*a(2)*d(3)+6*a(1)*d(4)-6*d(1)*a(4)-2*d(2)*a(3)))/24
d(6)=(15*Sc*tau*d(4)-Sc*(12*a(2)*d(4)-12*d(2)*a(4)+24*a(1)*d(5)-
24*d(1)*a(5)))/60;
b(5)=(K*(4*b(3)+24*a(5))+5*tau*b(3)+6*a(4)*b(1)+2*a(3)*b(2)-6*a(1)*b(4)-
2*a(2)*b(3))/(24*(1+K/2));
b(6)=(K*(12*b(4)+60*a(6))+18*b(4)*tau+24*a(5)*b(1)-24*a(1)*b(5)+12*a(4)*b(2)
-12*a(2)*b(4))/(60*(1+K/2));

%%%------------------------Matrix Creation-----------------------%%%

f=zeros(1,N);
h=zeros(1,N);
theta=zeros(1,N);
phi=zeros(1,N);
F=zeros(1,N);
H=zeros(1,N);
Theta=zeros(1,N);
Phi=zeros(1,N);
fs=zeros(1,N);
```

```
hs=zeros(1,N);
thetas=zeros(1,N);
phis=zeros(1,N);
Fs=zeros(1,N);
Hs=zeros(1,N);
Thetas=zeros(1,N);
Phis=zeros(1,N);

%%%%-------------Function values at first 5 mesh points-------------%%%

for i=1:5
    for j=1:6
        f(i)=f(i)+a(j)*(eps(i)^(j-1));
        h(i)=h(i)+b(j)*(eps(i)^(j-1));
        theta(i)=theta(i)+c(j)*(eps(i)^(j-1));
        phi(i)=phi(i)+d(j)*(eps(i)^(j-1));
    end
end
for i=1:5
    for j=1:5
        F(i)=F(i)+j*a(j+1)*((eps(i))^(j-1));
        H(i)=H(i)+j*b(j+1)*((eps(i))^(j-1));
        Theta(i)=Theta(i)+j*c(j+1)*((eps(i))^(j-1));
        Phi(i)=Phi(i)+j*d(j+1)*((eps(i))^(j-1));
    end
end

%%%%---------------Fourth-order Predictor-Corrector-----------------%%%

for j=5:N-1
    fs(j+1)=(-10*f(j)+18*f(j-1)-6*f(j-2)+f(j-3)+12*hstep*F(j))/3;
    hs(j+1)=(-10*h(j)+18*h(j-1)-6*h(j-2)+h(j-3)+12*hstep*H(j))/3;
    thetas(j+1)=(-10*theta(j)+18*theta(j-1)-6*theta(j-2)+theta(j-3)+
    12*hstep*Theta(j))/3;
```

```
phis(j+1)=(-10*phi(j)+18*phi(j-1)-6*phi(j-2)+phi(j-3)+12*hstep*Phi(j))/3
Fs(j+1)=(-1*(-30*(1+K)+20*f(j)*hstep-10*hstep*tau*eps(j+1)-
24*(hstep^2)*(tau+M))*F(j)+(8*(1+K)+36*f(j)*hstep-
18*hstep*tau*eps(j+1))*F(j-1)-(28*(1+K)+12*f(j)*hstep-
6*hstep*tau*eps(j+1))*F(j-2)+(12*(1+K)+2*f(j)*hstep-
hstep*tau*eps(j+1))*F(j-3)+2*(1+K)*F(j-4)+24*(hstep^2)*(F(j)^2-K*H(j)-
delta*theta(j)-delta1*phi(j)))/(20*(1+K)+6*hstep*f(j)-3*hstep*tau*eps(j+
F(j+1)=(-1*(30*(1+K)-96*f(j)*hstep-48*hstep*tau*eps(j+1)-
24*(hstep^2)*(tau+M))*F(j)+(8*(1+K)-72*f(j)*hstep+36*hstep*tau*eps(j+1))
-(28*(1+K)-32*f(j)*hstep+16*hstep*tau*eps(j+1))*F(j-2)+(12*(1+K)-6*f(j)*
+3*hstep+tau*eps(j+1))*F(j-3)+2*(1+K)*F(j-4)+24*(hstep^2)*((F(j)^2)-K*H(
-delta*theta(j)-delta1*phi(j)))/(20*(1+K)+50*hstep*f(j)-hstep*tau*eps(j+
Hs(j+1)=(-1*(10+12*hstep*(f(j)-0.5*tau*eps(j+1))/(1+0.5*K))*H(j)+18*H(j-
-6*H(j-2)+H(j-3)+(K*(3*F(j+1)+10*F(j)-18*F(j-1)+6*F(j-2)-F(j-3))+
12*hstep*(F(j)+1.5*tau+2*K)*h(j))/(1+0.5*K))/3;
Thetas(j+1)=(-1*(10*hstep+12*(hstep^2)*Pr*(f(j)-
0.5*tau*(eps(j+1)))/(1+4*R/3))*Theta(j)+18*hstep*Theta(j-1)-6*hstep*Thet
+hstep*Theta(j-3)-12*Pr*Ec*(1+K)*((F(j+1)/4+5*F(j)/6-3*F(j-1)/2+
F(j-2)/2-F(j-3)/12)^2)/(1+4*R/3)+12*(hstep^2)*(Pr*theta(j)*(F(j)+tau)-
Pr*M*Ec*(F(j)^2)-A1*F(j)-B1*theta(j))/(1+4*R/3))/(3*hstep);
Phis(j+1)=(-1*(10-6*hstep*tau*Sc*(eps(j+1))+12*hstep*Sc*f(j))*Phi(j)+
18*Phi(j-1)-6*Phi(j-2)+Phi(j-3)+12*hstep*phi(j)*Sc*(tau+F(j)))/3;
f(j+1)=(48*f(j)-36*f(j-1)+16*f(j-2)-3*f(j-3)+12*hstep*Fs(j+1))/25;
h(j+1)=(48*h(j)-36*h(j-1)+16*h(j-2)-3*h(j-3)+12*hstep*Hs(j+1))/25;
theta(j+1)=(48*theta(j)-36*theta(j-1)+16*theta(j-2)-3*theta(j-3)+
12*hstep*Thetas(j+1))/25;
phi(j+1)=(48*phi(j)-36*phi(j-1)+16*phi(j-2)-3*phi(j-3)+
12*hstep*Phis(j+1))/25;
H(j+1)=((48-12*hstep*(f(j)-0.5*tau*(eps(j+1))/(1+0.5*K)))*H(j)-
36*H(j-1)+16*H(j-2)-3*H(j-3)+(K*(25*F(j+1)-48*F(j)+36*F(j-1)-16*F(j-2)+
3*F(j-3))+12*hstep*(F(j)+1.5*tau+2*K)*h(j))/(1+0.5*K))/25;
Theta(j+1)=((48*hstep-12*(hstep^2)*Pr*(f(j)-0.5*tau*hstep*(j+2))/(1+4*R/
-36*hstep*Theta(j-1)+16*hstep*Theta(j-2)-3*hstep*Theta(j-3)-
12*Pr*Ec*(1+K)*((25*F(j+1)/12-4*F(j)+3*F(j-1)-4*F(j-2)/3+F(j-3)/4)^2)/(1
```

```
        12*(hstep^2)*(Pr*theta(j)*(F(j)+tau)-Pr*M*Ec*(F(j)^2)-A1*F(j)-
        B1*theta(j))/(1+4*R/3))/(25*hstep);
        Phi(j+1)=((48+12*hstep*tau*Sc*hstep*(j+2)-12*hstep*Sc*f(j))*Phi(j)-36*Ph
        16*Phi(j-2)-3*Phi(j-3)+12*hstep*phi(j)*Sc*(tau+F(j)))/25;
    end
    %if(k==1)
    %    F1=F(N);
    %end
    %if(k~=1)
    %    l1(k+1)=l1(k)-(l1(k)-l1(k-1))*F(N)/(F(N)-F1);
    %    err=abs(F(N));
    %    F1=F(N);
    %end

    %%%-------------------Serth's method----------------------%%%

    D=optimvar('D',4);   %% Lengendre Constants C
    xi=exp(-1*eps);      %% From serth's paper the transformation from eta to xi
    %syms f(xi);
    fun=S.*(D(1)+D(2)*(2.*xi-1)+D(3)*(6*power(xi,2)-6.*xi+1)+
    D(4)*(20*power(xi,3)-30*power(xi,2)+12.*xi-1));
    obj=sum((fun-f).^2);    %% Objective function
    lsqproblem=optimproblem("Objective",obj);
    x0.D=[3/2 1/2 3/2 1/2];
    [sol,fval] = solve(lsqproblem,x0);
    %err=evaluate(obj,sol);
    err=abs(f(N));
    x=evaluate(fun,sol);                    %% Updated error
    %figure(1)
    %plot(x);
    %hold on
    %plot(f);
    %responsedata = evaluate(fun,sol);
    %show(lsqproblem)
```

```
        fns = fieldnames(sol);
        %A.(fns{3})
        g=sol.(fns{1});
        syms y;
        func=S.*(g(1)+g(2)*(2.*y-1)+g(3)*(6*power(y,2)-6.*y+1)+
        g(4)*(20*power(y,3)-30*power(y,2)+12.*y-1));
        l(y)=diff(func);
        m(y)=diff(diff(func));
        %a=double(((l(exp(-xinf)))/m(exp(-xinf))));
        l1(k+1)=l1(k)-double(((l(exp(-xinf)))/m(exp(-xinf))));
        err=max([err,abs(h(N)),abs(theta(N)),abs(phi(N))]);

        %%%---------------Newton-Rhapson Method-------------------%%%

        l2(k+1)=l2(k)-h(N)/H(N);
        l3(k+1)=l3(k)-theta(N)/Theta(N);
        %l4(k+1)=l4(k)-phi(N)/Phi(N);
        l4(k+1)=l4(k);
        k=k+1;
end
Fi=smooth(F);
figure(2);
plot(eps,F);
%plot(eps,Fi,'b');
figure(3)
plot(eps,h);
figure(4)
plot(eps,theta);
figure(5)
plot(eps,phi);
```

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