Element-Free Simulation for Non-Newtonian Flows

L. Mai-Cao[1], T. Tran-Cong[2]

Summary

This paper presents a new element-free approach to the numerical analysis of non-Newtonian fluid flows. In this approach, the spatial discretization is based on the Indirect Radial Basis Function Networks (IRBFN) method where no element-based decomposition of the computation domain is required. High-order time discretization methods (Adams-Bashforth/Adams-Mouton) are used together within a three-step splitting scheme. A unified framework for the numerical analysis of generalized Newtonian fluid (GNF) and viscoelastic fluid flows is proposed and its implementation is verified.

Introduction

During the last twenty years, significant effort has been made to develop numerical methods for the simulation of viscoelastic fluid flows. In most cases, mixed finite element formulations are used in which, besides the velocity $\mathbf{v}$ and the pressure p, the extra stress τ is treated as an additional unknown. For the new approach presented in this paper, radial basis functions (RBFs) are used together with the collocation method for approximating functions and their derivatives whereas high-order time stepping schemes is used with the splitting technique for the temporal discretization. The idea of using radial basis functions (RBFs) for solving PDEs was first proposed in [2] and is hereby referred to as the Direct Radial Basis Function Network (DRBFN) method. Recently, a new method, namely the Indirect Radial Basis Function Network (IRBFN) was proposed in [5],[6] for the solution of differential equations and steady Navier-Stokes equations. In the DRBFN method, a function is first approximated by the RBFN and its derivatives are then calculated by differentiating such closed form RBFN approximant. In the IRBFN method, on the other hand, the highest derivative is first decomposed into radial basis functions. Lower derivatives and the function itself are then successively obtained via symbolic integrations. More recently, the method is extended to solve time dependent problems including those governed by parabolic, hyperbolic PDEs as well as convection-diffusion equations [4]. In this paper, time integration schemes are coupled with the IRBFN method by an extension of the splitting technique proposed in [3] for the Navier-Stokes equations.

[1]Faculty of Engineering and Surveying, University of Southern Queensland, Toowoomba, QLD 4350, Australia. E-mail: lanmai@usq.edu.au

[2]Corresponding author: Faculty of Engineering and Surveying, University of Southern Queensland, Toowoomba, QLD 4350, Australia. E-mail: trancong@usq.edu.au

Mathematical formulations

Consider an isothermal incompressible flows of a non-Newtonian fluid in a finite connected domain $\Omega \in \mathbb{R}^d,\ d = 2,3$. Let Γ_1 and Γ_2 be the two boundaries of Ω, $\Gamma_1 \cap \Gamma_2 = \varnothing$. The balance equations of mass and momentum can be written as

$$\nabla \cdot \mathbf{v} = 0, \tag{1}$$

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \eta_s \nabla^2 \mathbf{v} + \nabla\cdot\tau, \tag{2}$$

where ρ is the constant density, $\mathbf{v}$ the velocity field, p the pressure, η_s the solvent viscosity, and τ the non-Newtonian contribution to the total stress tensor.

The constitutive equation for GNF is given by

$$\tau = 2\eta_p \mathbf{d} - 2\eta_s \mathbf{d}, \tag{3}$$

where $\mathbf{d} = 1/2(\nabla\mathbf{v} + (\nabla\mathbf{v})^T)$ is the rate-of-strain tensor, $\eta_p = \eta_p(\dot{\gamma})$ is the viscosity as a function of $\dot{\gamma}$, the magnitude of the rate-of-strain tensor, $\dot{\gamma} = \sqrt{\mathbf{tr}(\mathbf{d}^2)}$. It should be noted that (2) is written in a generic non-Newtonian form that can be used for both GNF and viscoelastic fluids. As a result, (3) is modified so that (2) and (3) can express the momentum and constitutive equations as described in [1]. In the present work, two well-known models of GNF are considered. The first one is the power-law model given by

$$\eta = m\dot{\gamma}^{n-1}, \tag{4}$$

where n is the power-law exponent and m is another model parameter. The second one is the Carreau-Yasuda model given by

$$\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = [1 + (\lambda\dot{\gamma})^a]^{(n-1)/a} \tag{5}$$

where η_0 is the zero-shear-rate viscosity, η_∞ the infinitive shear rate viscosity, λ a time constant, a the dimensionless parameter representing the transition region between the zero-shear-rate region and the power-law region.

For the Oldroyd-B fluid, τ is defined by the constitutive law as follows [1]

$$\lambda\left(\frac{\partial \tau}{\partial t} + \mathbf{v}\cdot\nabla\tau - \tau\cdot\nabla\mathbf{v} - (\nabla\mathbf{v})^T\cdot\tau\right) + \tau = 2\eta_p\mathbf{d}, \tag{6}$$

where $\lambda > 0$ is the relaxation time, $\eta_p > 0$ the polymeric viscosity.

The above equations can be written in dimensionless form as follows

$$\nabla \cdot \mathbf{v} = \mathbf{0}, \tag{7}$$

$$Re\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}\right) = -\nabla p + \alpha \nabla^2 \mathbf{v} + \nabla \cdot \tau, \tag{8}$$

with the dimensionless constitutive equation for the viscoelastic (Oldroyd-B) fluid

$$We\left(\frac{\partial \tau}{\partial t} + \mathbf{v} \cdot \nabla \tau - \tau \cdot \nabla \mathbf{v} - (\nabla \mathbf{v})^T \cdot \tau\right) + \tau = (1-\alpha)\left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T\right), \tag{9}$$

or the constitutive law for the GNFs

$$\tau = 2\left(\beta \dot{\gamma}^{n-1} - 1\right)\mathbf{d} \quad \text{(Power-Law)}, \tag{10}$$

$$\tau = \left(2\left(1 + We^a \dot{\gamma}^a\right)^{(n-1)/a} + \frac{\eta_\infty}{\eta_r}\right)\mathbf{d} - 2\alpha\mathbf{d} \quad \text{(Carreau-Yasuda)}, \tag{11}$$

subject to initial and boundary conditions

$$\mathbf{v} = \mathbf{v}_{\Gamma_1} \quad \text{on } \Gamma_1, \qquad \mathbf{v}(0) = \mathbf{v}_0 \qquad \text{in } \Omega, \tag{12}$$

$$\tau = \tau_{\Gamma_2} \quad \text{on } \Gamma_2, \qquad \tau(0) = \tau_0 \qquad \text{in } \Omega \tag{13}$$

where the Reynolds number $Re = \rho VL/\eta_r$, the Weissenberg number $We = \lambda V/L$ in which V, L and $\eta_r V/L$ are characteristic velocity, length and stress, respectively. The ratio $\alpha = \eta_s/\eta_r$ where $\eta_r = \eta_s + \eta_p$ for viscoelastic fluids; $\eta_r = \eta_s$ for power-law fluids whereas $\eta_r = \eta_0 - \eta_\infty$ for Carreau-Yasuda fluids.

Time discretization

In this paper, the splitting scheme proposed in [3] is extended to deal with the non-Newtonian fluid by considering the stress tensor defined in the constitutive equation (9),(10) or (11) for the Oldroyd-B, Power-law or Carreau-Yasuda fluid, respectively, as the forcing term **f** in the Navier-Stokes equation. The incompressible Navier-Stokes equation is first integrated in time where the nonlinear advection term is approximated by the explicit Adams-Bashforth scheme and the linear diffusion term is discretized by the implicit Adams-Mouton scheme for stability improvement [3]. The resulting semi-discrete system can be then solved in the following three steps

Step 1

$$\frac{\tilde{\mathbf{v}}-\mathbf{v}^n}{\Delta t} = -\sum_{q=0}^{J_e-1} \beta_q (\mathbf{v}\cdot\nabla\mathbf{v})^{n-q} + \mathbf{f}^{n+1}, \tag{14}$$

Step 2a

$$\begin{aligned} \nabla^2 \overline{p}^{n+1} &= \frac{Re}{\Delta t}(\nabla\cdot\tilde{\mathbf{v}}), \qquad (15)\\ \frac{\partial \overline{p}^{n+1}}{\partial n} &= \mathbf{n}\cdot\left[-Re\sum_{q=0}^{J_e-1}\beta_q(\mathbf{v}\cdot\nabla\mathbf{v})^{n-q} - \alpha\sum_{q=0}^{J_e-1}\beta_q(\nabla\times(\nabla\times\mathbf{v}^{n-q}))\right], \end{aligned}$$

Step 2b

$$\frac{\hat{\mathbf{v}}-\tilde{\mathbf{v}}}{\Delta t} = -\frac{1}{Re}\nabla\overline{p}^{n+1}, \tag{16}$$

Step 3

$$\frac{\mathbf{v}^{n+1}-\hat{\mathbf{v}}}{\Delta t} = \frac{\alpha}{Re}\sum_{q=0}^{J_i-1}\gamma_q\nabla^2\mathbf{v}^{n+1-q}, \tag{17}$$

where J_e, J_i are the order of the explicit and implicit time integration schemes related to coefficients β_q and γ_q, respectively [3].

It should be noted that, at a given time step, the forcing term $\mathbf{f}^{n+1}$ is the divergence of the viscoelastic stress tensor which can be calculated by an explicit time integration scheme (e.g. Runge-Kutta, Adams-Bashforth) using the value of the velocity field from the previous step.

Space discretization by the IRBFN method

The semi-discrete system (14)-(17) is discretized in space by the IRBFN method. A function $u(\mathbf{x},t)$ and its derivatives can be approximated by the IRBFN method as follows [4]

$$u(\mathbf{x},t) \approx \psi^T(\mathbf{x})\boldsymbol{U}(t) = \sum_{i=1}^{M} U^{(i)}(t)\psi^{(i)}(\mathbf{x}), \tag{18}$$

$$u_{,j}(\mathbf{x},t) \approx \psi^T_{,j}(\mathbf{x})\boldsymbol{U}(t) \;=\; \sum_{i=1}^{M} U^{(i)}(t)\psi^{(i)}_{,j}(\mathbf{x}), \tag{19}$$

$$u_{,jj}(\mathbf{x},t) \approx \psi^T_{,jj}(\mathbf{x})\boldsymbol{U}(t) \;=\; \sum_{i=1}^{M} U^{(i)}(t)\psi^{(i)}_{,jj}(\mathbf{x}), \tag{20}$$

where M is the number of data points, $\boldsymbol{U}(t)$ the nodal values of function $u(\mathbf{x},t)$, and

$$\psi(\mathbf{x}) \;=\; \phi^T_j(\mathbf{x})\,\Phi_j^{-1}, \tag{21}$$

$$\psi_{,j}(\mathbf{x}) \;=\; \phi^T_{j,j}(\mathbf{x})\,\Phi_j^{-1}, \tag{22}$$

$$\psi_{,jj}(\mathbf{x}) \;=\; \phi^T_{j,jj}(\mathbf{x})\,\Phi_j^{-1}. \tag{23}$$

In the IRBFN method, $\phi_{j,jj}(\mathbf{x})$ is a given set of basis functions whose nonzero components can be chosen as multiquadrics $\phi^{(i)}_{j,jj}(\mathbf{x}) = \sqrt{r^{(i)^2} + s^{(i)^2}}$ or thin plate splines $\phi^{(i)}_{j,jj}(\mathbf{x}) = r^{(i)^{2m}} \log r^{(i)}$ where $r^{(i)}(\mathbf{x}) = ||\mathbf{x} - \mathbf{x}^{(i)}||$ is the Euclidian norm of vector $(\mathbf{x} - \mathbf{x}^{(i)})$. The lower derivative $\phi_{j,j}(\mathbf{x})$ and the function $\phi_j(\mathbf{x})$ in (22) and (21) can be then obtained via successive integrations of $\phi_{j,jj}(\mathbf{x})$ in j^{th} direction. It should be noted that the integration process gives rise to constants of integration which contribute to the formulations of $\phi_j(\mathbf{x})$ and $\phi_{j,j}(\mathbf{x})$ in (21)-(22) . The matrix Φ_j results from the application of $\phi_j(\mathbf{x})$ at every data points. More details on the IRBFN formulations for transient problems can be found in [4].

Numerical Examples

The present method performs well in simulating a number of non-Newtonian flows, including those of GNF and Oldroyd-B fluids. Due to lack of space only limited results are presented here in written form. In the simulation of the particle migration in concentrated suspensions, a GNF model is used as the constitutive equation for the particle flux. The concentration profile is investigated using the present approach and the steady state of the kinematics as well as the concentration profile are shown in Figure 1 where the numerical solution agrees well with the profile proposed in [7]. In another example is considered the numerical simulation of fluid flows in polymer processing. The problem is described as axisymmetric Poiseuille flow of Carreau-Yasuda fluid [1] (Figure 1). The start-up planar Poiseuille flow of the Oldroyd-B fluid whose velocity profiles at different times are shown in Figure 1 in comparison with the analytical solution from [8].

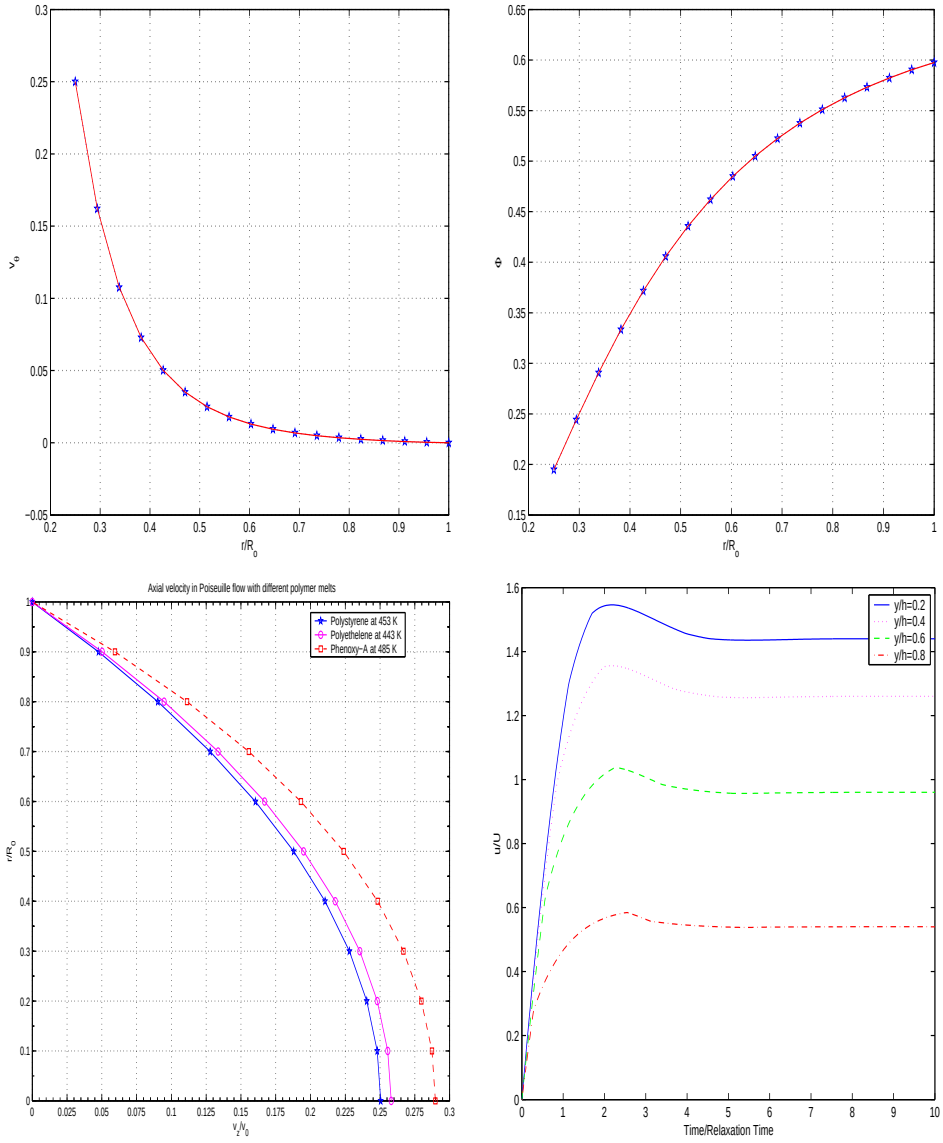

Figure 1: Suspension flow: velocity profile (top left), particle concentration profile (top right). Axisymmetric Poiseuille flow of polymer melts: velocity profile (bottom left). Start-up flow of the Oldroyd-B fluid: velocity profile (bottom right).

Conclusions

A new element-free approach to the numerical analysis of non-Newtonian fluid flows has been presented in this paper. The main feature of the approach is to combine high-order methods for time and space discretizations based on the IRBFN method and multistep time integration methods with the application of the operator splitting technique.

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