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BEM-RBF approach for viscoelastic flow analysis

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Abstract

A new BE-only method is achieved for the numerical solution of viscoelastic flows. A decoupled algorithm is chosen where the fluid is considered as being composed of an artificial Newtonian component and the remaining component is accordingly defined from the original constitutive equation. As a result the problem is viewed as that of solving for the flow of a Newtonian liquid with the non-linear viscoelastic effects acting as a pseudo body force. Thus the general solution is obtained by adding a particular solution to the homogeneous one. The former is obtained by a BEM for the base Newtonian fluid and the latter is obtained analytically by approximating the pseudo body force in terms of suitable radial basis functions (RBFs). Embedded in the approximation of the pseudo body force is the calculation of the polymer stress. This is achieved by solving the constitutive equation using RBF networks (RBFNs). Both the calculations of the particular solution and the polymer stress are therefore meshless and the resultant BEM-RBF method is a BE-only method. The complete elimination of any structured domain discretisation is demonstrated with a number of flow problems involving the Upper Convected Maxwell (UCM) and the Oldroyd-B fluids.

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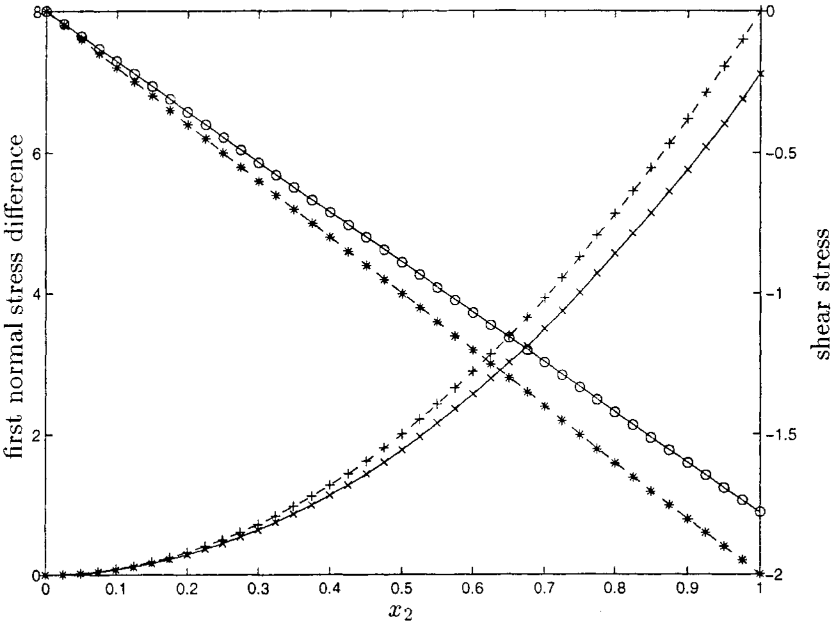

Figure 1: Planar Poiseuille flow of UCM and Oldroyd-B fluids at $W_e = 2.0$: The analytical solution, computed first normal stress difference and computed shear stress on the middle plane are denoted by {dashed line, +, *} and {solid line, ×, o} for UCM and Oldroyd-B fluids, respectively.

1 Introduction

The BEM has been successfully used in certain polymer flow analyses. However, the most direct transformation of differential equations governing nonlinear problems in continuum mechanics into equivalent integral equations usually retains volume integral terms. To make BEM generally competitive in comparison with FE-type numerical methods further improvements were effected by various techniques that help transform volume integrals into boundary integrals. These techniques include Dual Reciprocity Methods (DRM), Multiple Reciprocity Methods (MRM) and Particular Solution (PS). In most situations the volume integrals can only be replaced by boundary integrals in an approximate manner. In polymer flow analysis the complex constitutive relations for highly nonlinear viscoelastic materials present a challenge in numerical simulation where the solution of the constitutive equation is a difficult task on its own in additional to the transformation of the volume integrals. In the case of viscoelastic materials the constitutive

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equations for extra stresses are also partial differential equations (differential models) to be solved. This paper presents a BEM-RBF formulation that results in a BE-only numerical method for viscoelastic flows.

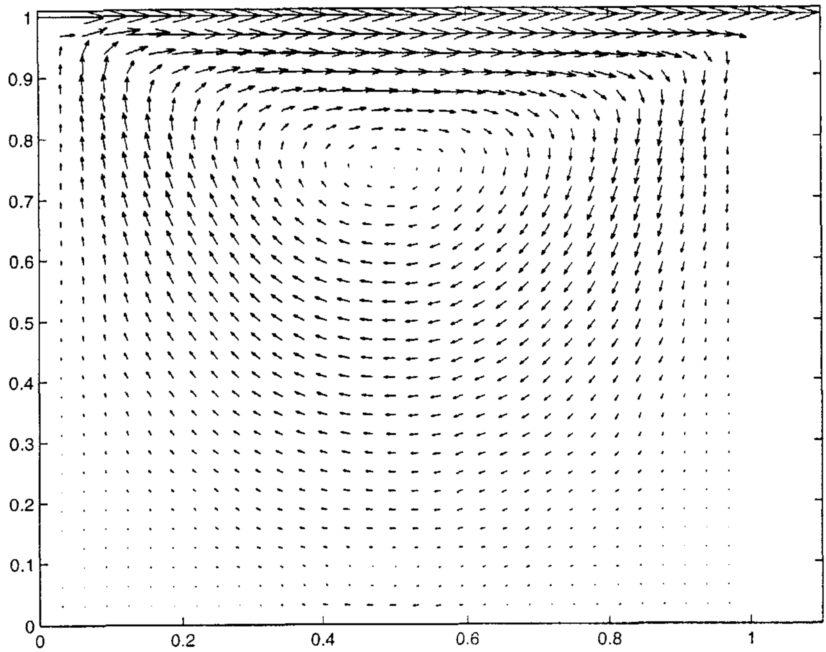

Figure 2: Driven cavity flow of Oldroyd-B fluid: velocity field at $W_e = 0.1$.

2 Governing Equations

The flow is assumed to be isothermal, creeping, and incompressible for which the equations of motion are

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \mathbf{x} \in V, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \quad \mathbf{x} \in V, \tag{2}$$

where $\boldsymbol{\sigma}$ is the total stress tensor and $\mathbf{u}$ is the velocity vector. For Oldroyd-B model, the total stress tensor $\boldsymbol{\sigma}$ can be written as

$$\boldsymbol{\sigma} = -P\mathbf{1} + 2\eta_s \mathbf{D} + \boldsymbol{\tau} \tag{3}$$

where P is the pressure, $\mathbf{1}$ is the unit tensor, η_s is the "Newtonian contribution" viscosity, $\mathbf{D}$ is the rate of strain tensor and $\boldsymbol{\tau}$ is the extra stress

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tensor obeying

$$\lambda \frac{\triangle \boldsymbol{\tau}}{\triangle t} + \boldsymbol{\tau} = 2\eta_p \mathbf{D} \tag{4}$$

in which λ is the relaxation time, η_p is the "polymer contribution" viscosity and $\frac{\triangle \boldsymbol{\tau}}{\triangle t}$ is the upper convected derivative of $\boldsymbol{\tau}$ defined by

$$\frac{\triangle \boldsymbol{\tau}}{\triangle t} = \frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\tau} - \nabla \boldsymbol{\tau} \cdot \mathbf{u} - \boldsymbol{\tau} \cdot \nabla \mathbf{u}^T \tag{5}$$

In the Oldroyd-B model the parameter λ is related to the material retardation time via $\bar{\lambda} = \alpha\lambda$, where $\alpha = \eta_s/(\eta_s + \eta_p)$. For a UCM fluid $\eta_s = 0$ and (3) is rewritten as

$$\boldsymbol{\sigma} = -P\mathbf{1} + 2\eta_n \mathbf{D} + (\boldsymbol{\tau} - 2\eta_n \mathbf{D}), \tag{6}$$

where η_n is a conveniently chosen viscosity. In this work $\eta_n = \eta_p$ is chosen. To facilitate the general discussion applicable to both model fluids, the governing equations are now written as

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^N + \boldsymbol{\varepsilon}, \tag{7}$$

$$\boldsymbol{\sigma}^N = -P\mathbf{1} + 2\eta\mathbf{D}, \tag{8}$$

$$\nabla \cdot \boldsymbol{\sigma}^N = \mathbf{B}, \tag{9}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{10}$$

where $\mathbf{B} = -\nabla \cdot \boldsymbol{\varepsilon}$; and $\eta = \eta_s$, $\boldsymbol{\varepsilon} = \boldsymbol{\tau}$ for the Oldroyd-B model and $\eta = \eta_n$, $\boldsymbol{\varepsilon} = \boldsymbol{\tau} - 2\eta_n \mathbf{D}$ for the UCM model.

3 BEM-RBF formulation

The constitutive equation for extra stress (4) must be solved in conjunction with the equations of motion (1) and (2). The unknown fields are the polymer stress $\boldsymbol{\tau}$, the velocity $\mathbf{u}$ and the pressure P. Rewriting the governing equations as (7)-(10) allows us to view the problem as one involving a Newtonian liquid defined by (8) with a pseudo body force defined by $\mathbf{B} = -\nabla \cdot \boldsymbol{\varepsilon}$. Therefore a decoupled technique is employed here to break the problem down into two stages: the solution of an elliptic Newtonian-like flow (9) and (10) and the solution of the constitutive model (4). The two stages constitute a Picard-type iterative scheme where the pseudo body force is assumed known from the previous iteration. The first stage is solved by a BEM and the second is solved by radial basis function networks (RBFN). The iterative procedure is terminated at the iteration k when

$$CM = \sqrt{\frac{\sum_{j=1}^{n}\sum_{i=1}^{3}(u_i^{(j)(k)} - u_i^{(j)(k-1)})^2}{\sum_{j=1}^{n}\sum_{i=1}^{3}(u_i^{(j)(k-1)})^2}} < tol \tag{11}$$

where CM is regarded as convegence measure, n is number of data points and tol is a preset tolerance which is set at $5.e-3$ in the present work.

3.1 Direct integral equation formulation

The details of the process of recasting the set of governing equations into integral form are given elsewhere (e.g. [1-2]) and the final IE is given by

$$C_{ij}(\mathbf{x})u_j(\mathbf{x}) = \int_{\partial V} u^*_{ij}(\mathbf{x},\mathbf{y})t_j(\mathbf{y})d\Gamma(\mathbf{y}) - \int_{\partial V} t^*_{ij}(\mathbf{x},\mathbf{y})u_j(\mathbf{y})d\Gamma(\mathbf{y}) - \int_V \varepsilon_{jk}(\mathbf{y})\frac{\partial u^*_{ij}(\mathbf{x},\mathbf{y})}{\partial x_k}d\Omega(\mathbf{y}), \quad (12)$$

where V is the solution domain of the problem with boundary ∂V; $\mathbf{x},\mathbf{y} \in V$; $u_j(\mathbf{y})$ is the j component of the velocity at $\mathbf{y}$; $t_j(\mathbf{y})$ is the j component of boundary traction at $\mathbf{y}$; $\varepsilon_{jk}(\mathbf{y})$ is the jk component of $\boldsymbol{\varepsilon}$ at $\mathbf{y}$; $u^*_{ij}(\mathbf{x},\mathbf{y})$ is the i component of velocity field at $\mathbf{x}$ due to a point force in j direction at $\mathbf{y}$ (Kelvin fundamental solution) and $t^*_{ij}(\mathbf{x},\mathbf{y})$ is its associated traction. $C_{ij}(\mathbf{x})$ depends on local geometry, $C_{ij}(\mathbf{x}) = \delta_{ij}$ if $\mathbf{x} \in V$ and $C_{ij}(\mathbf{x}) = \frac{1}{2}\delta_{ij}$ if $\mathbf{x} \in \partial V$ and ∂V is a Liapunov surface.

3.2 Elimination of volume integral by PS techniques

The elementary process of numerically evaluating the volume integral in (12) normally requires some kind of volume discretization. This element-based numerical integration can be avoided by using the PS technique (e.g. [3-5]). In the present technique, the total solution to (9)-(10) is decomposed into the homogeneous part and a particular solution as

$$\mathbf{u} = \mathbf{u}^H + \mathbf{u}^P, \quad (13)$$

$$\boldsymbol{\sigma}^N = \boldsymbol{\sigma}^H + \boldsymbol{\sigma}^P. \quad (14)$$

Note that the solution $\mathbf{u}$ to (9)-(10) is also the solution to the original problem and therefore the superscript ^{N} is not necessary. At this point, it is more convenient to consider the equivalent elasticity problem in obtaining a particular solution and the corresponding solution for the incompressible Newtonian liquid is obtained by allowing $\nu \to 1/2$ in the final results and reinterpreting displacement as velocity. Thus the Navier's equation for a particular solution is considered and given by

$$\frac{\eta}{1-2\nu}\nabla\nabla\cdot\mathbf{u}^P + \eta\nabla^2\mathbf{u}^P = \mathbf{B}, \quad (15)$$

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where ν is the Poisson's ratio and η the shear modulus. A particular solution of (15) for displacement u_i^P and the corresponding stress σ_{ij}^P are given in terms of the Galerkin vector (e.g. [6]) by

$$u_i^P = G_{i,kk} - \frac{1}{2(1-\nu)} G_{k,ik} \quad (16)$$

$$\sigma_{ij}^P = \frac{\eta}{1-\nu} \left[\nu G_{k,nnk} \delta_{ij} - G_{k,ijk} + (1-\nu)(G_{i,jkk} + G_{j,ikk}) \right] \quad (17)$$

where G_i is the Galerkin vector which is the solution to the following biharmonic equation

$$\eta \nabla^4 G_i = \mathbf{B}. \quad (18)$$

To solve (18) approximately, the pseudo-body force term $\mathbf{B}$ is decomposed into suitable radial basis functions and the final solution for u_i^P and stress σ_{ij}^P were given in [7]. The homogeneous solution to (9) and (10) is obtained via a BEM derived from the equivalent boundary integral form

$$C_{ij}(\mathbf{x}) u_j^H(\mathbf{x}) = \int_{\partial V} u_{ij}^*(\mathbf{x}, \mathbf{y}) t_j^H(\mathbf{y}) d\Gamma(\mathbf{y}) - \int_{\partial V} t_{ij}^*(\mathbf{x}, \mathbf{y}) u_j^H(\mathbf{y}) d\Gamma(\mathbf{y}), \quad (19)$$

where the boundary conditions are determined by

$$u_i^H = u_i - u_i^P \quad (20)$$

$$\sigma_{jk}^H = \sigma_{jk}^N - \sigma_{jk}^P = \sigma_{jk} - \varepsilon_{jk} - \sigma_{jk}^P \quad (21)$$

Substitution of (20) and the traction obtained from (21) into (19) yields

$$\begin{aligned} C_{ij}(\mathbf{x}) u_j(\mathbf{x}) = & \int_{\partial V} u_{ij}^*(\mathbf{x}, \mathbf{y}) t_j(\mathbf{y}) d\Gamma(\mathbf{y}) - \int_{\partial V} t_{ij}^*(\mathbf{x}, \mathbf{y}) u_j(\mathbf{y}) d\Gamma(\mathbf{y}) \\ & - \int_{\partial V} u_{ij}^*(\mathbf{x}, \mathbf{y}) t_j^\varepsilon(\mathbf{y}) d\Gamma(\mathbf{y}) + C_{ij}(\mathbf{x}) u_j^P(\mathbf{x}) \\ & - \int_{\partial V} u_{ij}^*(\mathbf{x}, \mathbf{y}) t_j^P(\mathbf{y}) d\Gamma(\mathbf{y}) + \int_{\partial V} t_{ij}^*(\mathbf{x}, \mathbf{y}) u_j^P(\mathbf{y}) d\Gamma(\mathbf{y}) \end{aligned} \quad (22)$$

where u_j and t_j are the velocity and the total traction, respectively. Note that by using the fixed kinematics obtained from the previous iteration, the pseudo body force term and the corresponding particular solution are known at the current iteration. Hence, the unknowns in the final equation (22) which contains only boundary integrals are the velocity and the total boundary traction. At this stage, it can be seen that the volume integral has been eliminated. We note, however, that the gradients of the stress and the velocity still exist in (18) and (4), respectively. Previously these gradients have been computed via the derivatives of the assumed shape functions of the finite elements representing the domain. It is part of the aim of this paper to show that we can compute these gradients without discretising

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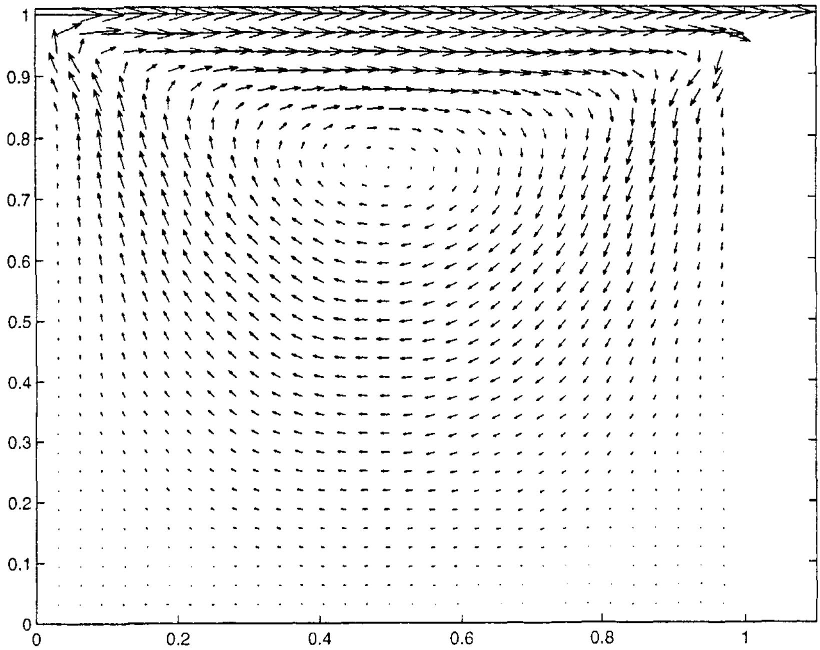

Figure 3: Driven cavity flow of Oldroyd-B fluid: velocity field at $W_e = 0.15$.

the domain into structured finite elements by using neural networks such as RBFN. Furthermore, the constitutive equation for extra stress is also solved by a meshless RBFN method as described in the next section

3.3 RBFN for the solution of constitutive model

The function is decomposed into weighted radial basis functions in which each radial basis function contains the center and the width parameters. In order to keep the mathematics simple (only linear algebra), these parameters are chosen in advance and the unknowns therefore are RBFN weights only. The network only needs an unstructured distribution of collocation points throughout the volume for approximation and hence the need for discretisation of the volume of the analysis domain into a set of finite elements is eliminated. It should be noted here that although RBFN theoretically have an ability to represent any continuous function to a prescribed degree of accuracy, they cannot practically acquire sufficient approximation accuracy in most cases. The so called indirect approach (IRBFN) appears to be superior among alternative RBFN approaches for function approximation over a set of noiseless data points and for numerical solution of PDE [8-9]. This IRBFN approach is therefore employed in the present work. In the case of numerical solution of the constitutive equation (4), each variable τ_{ij} is represented by an IRBFN. The kinematics assumes the value obtained in the first part of the iteration. Then the training processes for networks are employed simultaneously by minimizing the following sum squared error

$$SSE =$$
$$\sum_{i=1}^{n}\left[(1-2\lambda u_{1,1}^{(i)})\tau_{11}^{(i)}+\lambda u_1^{(i)}\tau_{11,1}^{(i)}+\lambda u_2^{(i)}\tau_{11,2}^{(i)}-2\lambda u_{1,2}^{(i)}\tau_{12}^{(i)}-2\eta_p u_{1,1}^{(i)}\right]^2+$$
$$\sum_{i=1}^{n}\left[-\lambda u_{2,1}^{(i)}\tau_{11}^{(i)}+\tau_{12}^{(i)}+\lambda u_1^{(i)}\tau_{12,1}^{(i)}+\lambda u_2^{(i)}\tau_{12,2}^{(i)}-\lambda u_{1,2}^{(i)}\tau_{22}^{(i)}-\eta_p(u_{1,2}^{(i)}+u_{2,1}^{(i)})\right]^2$$
$$+\sum_{i=1}^{n}\left[-2\lambda u_{2,1}^{(i)}\tau_{12}^{(i)}+(1-2\lambda u_{2,2}^{(i)})\tau_{22}^{(i)}+\lambda u_1^{(i)}\tau_{22,1}^{(i)}+\lambda u_2^{(i)}\tau_{22,2}^{(i)}-2\eta_p u_{2,2}^{(i)}\right]^2$$
$$+\sum_{i=1}^{n}[\tau_{11}-\bar{\tau}_{11}]^2+\sum_{i=1}^{n}[\tau_{12}-\bar{\tau}_{12}]^2+\sum_{i=1}^{n}[\tau_{22}-\bar{\tau}_{22}]^2 \qquad (23)$$

where n is the number of colocation points (also the number of centres here), τ_{ij} and $\bar{\tau}_{ij}$ are the polymer stress obtained by symbolically integrating $\tau_{ij,11}$ and $\tau_{ij,22}$ respectively. Note that if the boundary conditions for the polymer stress τ_{ij} exist, the above SSE will also contain error terms corresponding to these boundary conditions.

4 Planar Poiseuille Flow

The problem of planar Poiseuille flow of UCM and Oldroyd-B ($\alpha = 1/9$) fluids has an analytical solution given by

$$u_1 = U\left[1-\left(\frac{x_2}{L}\right)^2\right], \quad u_2 = 0 \qquad (24)$$

$$\tau_{11} = 2\lambda\eta_p\left(\frac{\partial u_1}{\partial x_2}\right)^2, \quad \tau_{12}=\eta_p\frac{\partial u_1}{\partial x_2}, \quad \tau_{22}=0 \qquad (25)$$

where U is the maximum speed, L is one half of the width of the chanel and x_1-axis is chosen to coincide with the centreline. Owing to symmetry, only one half of the fluid domain is considered with the dimension being $L \times L$. The maximum speed U and the width L are taken to be units. At the inlet and the outlet, Dirichlet boundary conditions for the velocity and Neumann boundary conditions for the extra stress are imposed. No-slip conditions are enforced on the solid boundary and symmetry conditions are specified on the plane of symmetry. The Weissenberg number W_e is defined by $W_e = \lambda\dot{\gamma}$ where $\dot{\gamma}$ is the shear rate at the wall. It is observed that RBFNs are able to represent the numerical solution of (4) using relative lower centre density. Using 160 linear boundary elements for the BEM, 41×41 centres for the approximation of the PS and a centre density 11×11 for RBFN for polymer stress, the present method achieves up to $W_e = 10$ for both UCM and Oldroyd-B models. The simulation is arbitrarily stopped at $W_e = 10$ for lack of interest. The stress obtained at $W_e = 2$ on a middle plane is displayed in Figure 1 showing good agreement with the analytical solution.

5 2D Driven Square Cavity Flow

One of the benchmark problems for viscous fluids is the lid-driven cavity flow. However, for viscoelastic fluids there are very few numerical results reported [10-12], which are all based on finite element methods. The present results cannot be compared directly with those just cited due to the different model fluids used in each case. However, the general behaviour of the flow field, including the core vortex, is in agreement with the experimental result using an ideal elastic Boger fluid [13] (Figures 2-3.) In the above figures the results are obtained using 128 linear BEs, 33×33 centres for PS, and 17×17 centres for polymer stress. The Weissenberg number is $W_e = \lambda U/L$ where U is the speed of the lid, L is the size of the square cavity and λ is the material time constant of the Oldroyd-B fluid with $\alpha = 1/9$. The centre of the core vortex shifts progressively upstream as the W_e number increases. This is in contrast with the Newtonian results where the vortex shifts downstream as the Re number increases.

6 Concluding Remarks

This work demonstrates the successful implementation of two new key ideas of formulating the viscoelastic flow problems in terms of boundary integral only via the use of particular solution and the solution of the constitutive equation for polymer stress using RBFNs. The ideas are not restricted to viscoelastic flows and can be applied to other problems governed by PDEs.

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