Decoupled Spectral Element Methods for Steady Viscoelastic Flow Past a Sphere

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Abstract

A spectral element method is described for the flow of a viscoelastic fluid past a sphere in a tube. An approximate Jacobian is used to solve the system of nonlinear algebraic equations derived from the spectral element discretization as a cost-effective alternative to the full Newton method. The linearized equations are solved using a preconditioned generalised minimal residual (GMRES) method. Numerical results showing the behaviour of the drag on the sphere as a function of the elasticity of the fluid are presented. A comparison with other methods is made and shows good agreement with the results of the proposed method.

Key words: viscoelastic flow, drag factor, spectral elements, GMRES method.

AMS subject classifications: 76A10, 76M25, 65F10, 65N35.

1 Introduction

The mathematical solution for the flow field generated by a particle moving at low speed through an infinite expanse of Newtonian fluid was produced by Stokes [24] as long ago as 1851. The problem of determining the influence of the walls of a nearby container on the drag force experienced by the particle was not solved until much later. The determination of the drag force, or equivalently the settling velocity, of a spherical particle in a viscoelastic fluid has attracted much attention in recent years for a number of reasons. The first concerns the experimentally observed changes in behaviour from Newtonian flow. Jones *et al* [14] investigated experimentally the dependence of the normalised drag on the sphere on the Deborah number and on the ratio β of the radius of the sphere to that of the containing cylinder. Their experiments with a maltose syrup/water based Boger fluid and a Newtonian fluid of equivalent viscosity showed that a substantially higher drag could be observed for the Boger fluid in the limiting cases of β very small or almost unity. Much smaller drag values were observed for some intermediate values of β. Secondly, there is the practical importance of the problem as seen in its use as a simple rheological test for industrial fluids (see [1], for example). Thirdly, the problem is useful in gaining insights into settling in particle suspensions. Finally, this problem has been chosen as a benchmark problem in computational rheology [12] for the comparison of different numerical methods since it generates a complex flow field without introducing the problems associated with corner singularities.

At the present time finite element methods, streamline upwinded finite element methods and boundary element methods (see [5], [8], [13], [15], [21], [25], [30] for example) have been used to solve the system of coupled non-linear partial differential equations that arise from viscoelastic flow problems, and good agreement has been obtained albeit for small (< 2.0) values of the Deborah number when the Maxwell and Oldroyd B constitutive models have been used. In 1994, Debae *et al* [9] did a comparison of four stress-velocity-pressure algorithms to calculate solutions to benchmark problems, including that of the flow of a Maxwell fluid around a sphere. These algorithms were tested with three different methods of integration of the constitutive equations: the Streamline-Upwinded/Petrov-Galerkin (SUPG) and Streamline-Upwind (non-consistent) (SU) methods introduced by Brooks and Hughes [4], as well as a Galerkin method. In the Galerkin formulation the largest Deborah numbers were obtained for the Elastic-Viscous Split Stress (EVSS) method of Rajagopalan *et al* [20].

The application of spectral methods to viscoelastic flow problems is comparatively recent, having first been used in this way in 1987 by Beris *et al* [3] to solve the flow of

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a Maxwell fluid through eccentrically rotating cylinders. Since this time spectral methods have enjoyed extensive application to viscoelastic flow problems. The importance of the present paper is in its contribution to the growing literature on the numerical simulation of viscoelastic flow past a sphere in a cylinder and the opportunity that this presents for a comparison of spectral methods with other numerical techniques. The use of spectral methods with domain decomposition techniques combines the flexibility of the finite element method with highly-accurate spectral methods. The spectral element method is based on a variational formulation of the problem in which the integrals are approximated using Gaussian quadrature rules. The choice of compatible velocity and pressure approximation spaces ensures that there are no spurious modes in the pressure representation. Spectral element methods have been used in the viscoelastic context by Van Kemenade and Deville [27] who compared the results of their spectral element method with the 4×4 SUPG finite element method on the perturbed channel flow problem with a Maxwell B fluid. Their spectral element method was also compared with other numerical methods for the flow of the Maxwell B fluid in a wavy tube. In another paper, Van Kemenade and Deville [28] compared their method with the EVSS method on slightly perturbed viscometric flows in a channel. They found that the computational cost of the spectral element method was less than for the EVSS method. The method was also used to study flow resistance in a periodically constricted tube. Spectral element methods were used recently by the present authors [18] in order to solve for the flow of an Oldroyd B fluid past a sphere in a tube.

Numerical methods for solving viscoelastic flow problems may be divided into two classes - coupled and decoupled methods. In the coupled approach the system of partial differential equations is linearised using Newton's method. The linearised equations are discretised and then solved simultaneously using a sparse matrix solver, for example. In the decoupled approach time-splitting methods are generally used to march the system forward in time to a steady state solution, if one exists. Decoupled methods have the advantage of being able to solve problems with finer discretisations since they break the problem down into a number of smaller subproblems. They are ideal, therefore, for simulating computationally intensive 3-D transient flows. Coupled methods are prohibitively expensive for these types of problem. The disadvantage of decoupled methods would seem to be that, at least at the present time, it is not possible to reach as high a limiting value of the Deborah number as for corresponding coupled methods.

The main disadvantage of Newton's method, seen particularly in three dimensional applications, is the size of the Jacobian matrix that needs to be computed at each step. As a cost effective alternative to the full Newton method the present paper uses a modified generalised minimal residual (GMRES) method and this is explained in section 4. The GMRES method was originally proposed by Saad and Schultz [22] and developed for viscoelastic flow simulations by Fortin and Zine [10]. The method is used with an approximate Jacobian in each Newton step and allows us to decouple the computation of the velocity and pressure from that of the stress tensor. The time splitting method originally proposed by Chorin [7] and Temam [26] and used by the present authors in conjunction with spectral elements for the flow of an Oldroyd B fluid past a sphere in a cylinder (see [17], [18]) is outlined in section 3. This latter scheme completely decouples the velocity and pressure computations. The upper bound encountered on the Deborah number De in [17] and [18] was approximately 0.6 and this is typical of decoupled methods. The results from the GMRES method are compared with those obtained in [18] in section 5.

2 Geometry and governing equations

The governing equations are those of continuity, momentum and the constitutive equation for the stresses. Within a flow of a fluid of Maxwell or Oldroyd type, with velocity everywhere finite, there may exist infinite stresses exerted by supposedly infinitely extended polymers. In the numerical simulations using these models a build up of large polymer extensions may be observed which gives rise to large elastic stresses and eventual numerical breakdown. The difficulty of infinite extensibility may be obviated by using, for example, the Chilcott-Rallison constitutive model [6] which incorporates a finite degree of extensibility for the polymers. In this model a single parameter, the maximum extensibility of the dumbbells, L, controls the plateau of the extensional viscosity at high extension rates.

The equations of motion and continuity for unsteady, inertialess flow are

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\nabla p + \eta_2 \nabla^2 \mathbf{v} + \nabla \cdot \frac{\eta_1 f(R)}{\lambda_1} (\mathbf{A} - \mathbf{I}), \tag{1}$$

$$\nabla \cdot \mathbf{v} = 0, \tag{2}$$

where p is an arbitrary isotropic pressure, η_1 is a polymeric viscosity, η_2 is a solvent viscosity, λ_1 is a characteristic relaxation time for the fluid, ρ is the fluid density, $\mathbf{v}$ is the

velocity vector and the tensor $\mathbf{A}$ represents an ensemble average over the distribution space of the dyadic product $\mathbf{RR}$ of the dumbbell configuration vector $\mathbf{R}$. The function $f(R)$ is a nonlinear force law, dependent upon the length, R. of the dumbbell configuration vector.

The evolution equation for $\mathbf{A}$ is

$$\mathbf{A} + \frac{\lambda_1}{f(R)}\mathbf{A}_{(1)} = \mathbf{I}, \tag{3}$$

where the subscript "(1)" in (3) denotes the upper-convected derivative.

The problem geometry is shown in Fig.1. A rigid sphere of radius a falls with terminal velocity U along the centreline of a cylindrical tube of radius R. In the numerical simulation of this problem it is assumed that the flow is axisymmetric and creeping and that the sphere is motionless with the tube wall moving with speed U instead.

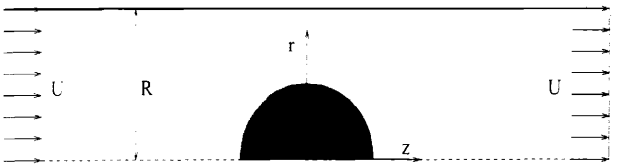

Figure 1: The problem geometry

The Deborah number for this problem is defined by

$$De = \frac{\lambda_1 U}{a}.$$

The nonlinear set of equations (1),(2),(3) is the one that is solved.

3 A time splitting scheme.

Time splitting schemes have the advantage of enabling the different operators in a system of partial differential equations to be treated by appropriate methods of solution. In the present context time splitting methods are used as a means of determining the solution of the corresponding steady problem. In this respect they may be viewed as iterative techniques. In general, nonlinear operators such as the convection operator are treated explicitly while linear operators such as the diffusion, gradient and divergence operators may be treated implicitly.

The four components of the constitutive equation (3) are discretised in time using the backward Euler scheme on the full system of equations by freezing the velocity field at the previous time step. In order to solve the momentum and continuity equations the time-splitting or projection scheme of Chorin [7] and Temam [26] is used. This scheme completely decouples the diffusion and pressure computations. The diffusion term is treated implicitly in the current formulation. The pressure is determined so that the velocity field at the end of the current time step is divergence-free in a weak sense.

The superscript on a variable denotes the time increment. We denote by Δt the time step. Let $(\mathbf{v}^0, p^0, \mathbf{A}^0)$ be the initial approximation at time $t = 0$. The approximation at time $t = (n+1)\Delta t$ is determined from the approximation $(\mathbf{v}^n, p^n, \mathbf{A}^n)$ at the previous time $t = n\Delta t$ by the following scheme:

Stage 1.

$$(1 + \frac{\Delta t f(R)}{\lambda_1})\mathbf{A}^{n+1} + \Delta t\,(\mathbf{v}^n \cdot \nabla \mathbf{A}^{n+1} - \nabla \mathbf{v}^n \cdot \mathbf{A}^{n+1} - \mathbf{A}^{n+1} \cdot (\nabla \mathbf{v}^n)^T) = 2\eta_1 \frac{\Delta t f(R)}{\lambda_1}\mathbf{I} + \mathbf{A}^n, \tag{4}$$

Stage 2.

$$\rho(\frac{\mathbf{v}^* - \mathbf{v}^n}{\Delta t}) = \nabla \cdot \frac{\eta_1 f(R)}{\lambda_1}(\mathbf{A}^n - \mathbf{I}), \tag{5}$$

Stage 3a.

$$\rho(\frac{\mathbf{v}^{n+1} - \mathbf{v}^*}{\Delta t}) = -\nabla p^{n+1} + \eta_2 \nabla^2 \mathbf{v}^{n+1}, \tag{6}$$

Stage 3b.

$$\nabla \cdot \mathbf{v}^{n+1} = 0. \tag{7}$$

The spectral element method is applied to Stage 3 of the backward Euler scheme. The velocity field is chosen to belong to the space $X = H_0^1(\Omega) \times H_0^1(\Omega)$ and the pressure to the space $L^2(\Omega)$. The variational formulation of (6)-(7) is therefore: Find $(\mathbf{v}, p) \in X \times L^2(\Omega)$, such that

$$\iint_\Omega (\eta_2(\nabla \mathbf{v})^T : \nabla \mathbf{w}) r\,dr\,dz + \frac{\rho}{\Delta t}\iint_\Omega (\mathbf{v} \cdot \mathbf{w}) r\,dr\,dz - \iint_\Omega (p \nabla . \mathbf{w}) r\,dr\,dz = \frac{\rho}{\Delta t}\iint_\Omega (\mathbf{v}^* . \mathbf{w}) r\,dr\,dz, \quad \forall\, \mathbf{w} \in X, \tag{8}$$

$$\iint_\Omega (\nabla \cdot \mathbf{v} q) r\,dr\,dz = 0,\ \forall\, q \in L^2(\Omega), \tag{9}$$

where we have dropped the time level $n+1$ from the superscript on $\mathbf{v}$ and p. The vector of test functions $\mathbf{w}$ is taken to be either $(w_r, 0)$ or $(0, w_z)$ where w_r and w_z are test functions in $H_0^1(\Omega)$.

4 A modified GMRES method.

The variational formulation for the steady form of (1)-(3) is: Find $(\mathbf{v}, p, \mathbf{A}) \in X \times L^2(\Omega) \times L_A(\Omega)$, such that

$$\int\int_\Omega (\eta_2(\nabla \mathbf{v})^T : \nabla \mathbf{w}) r \, dr \, dz - \int\int_\Omega (p \nabla \cdot \mathbf{w}) r \, dr \, dz = -\frac{\eta_1}{\lambda_1} \int\int_\Omega (f(R)(\mathbf{A} - \mathbf{I}) : \nabla \mathbf{w}) r \, dr \, dz, \quad \forall \, \mathbf{w} \in X, \tag{10}$$

$$\int\int_\Omega (\nabla \cdot \mathbf{v} q) r \, dr \, dz = 0, \ \forall \, q \in L^2(\Omega), \tag{11}$$

$$\int\int_\Omega \left(\mathbf{A} + \frac{\lambda_1}{f(R)} \mathbf{A}_{(1)} \right) : \phi r \, dr \, dz = \int\int_\Omega \mathbf{I} : \phi r \, dr \, dz, \quad \forall \phi \in L_A(\Omega), \tag{12}$$

where $L_A(\Omega)$ is the space of symmetric tensors whose components are square integrable.

For a given tensor $\mathbf{A}$ equations (10) and (11) represent a steady Stokes problem. The solution of this problem may then be regarded as a function of $\mathbf{A}$, i.e. the velocity $\mathbf{v}$ and the pressure p depend on $\mathbf{A}$. Therefore, we can write (12) in the matrix form

$$\mathbf{E}_{\mathbf{v}(\mathbf{A})} \mathbf{A} = \mathbf{b}_{\mathbf{v}(\mathbf{A})}, \tag{13}$$

where the subscript $\mathbf{v}(\mathbf{A})$ indicates that the matrix $\mathbf{E}$ and the right hand side vector $\mathbf{b}$ depend upon $\mathbf{v}$. This is a nonlinear system of equations for $\mathbf{A}$. We can write this system in the form

$$\mathbf{F}(\mathbf{A}) = \mathbf{0},$$

and then solve it using Newton's method:

1. Let $\mathbf{A}_0$ be an initial guess.
2. For $n \geq 0$, solve $\mathbf{J}_n \delta \mathbf{A} = -\mathbf{F}(\mathbf{A}_n)$
3. Set $\mathbf{A}_{n+1} = \mathbf{A}_n + \delta \mathbf{A}$
4. Continue until convergence.

In the above $\mathbf{J}_n$ is the Jacobian matrix of $\mathbf{F}$.

The GMRES method is applied to the solution of step 2 for $\delta \mathbf{A}$:

$$\mathbf{J}_n \delta \mathbf{A} = -\mathbf{F}(\mathbf{A}_n). \tag{14}$$

Rather than compute and store the full Jacobian $\mathbf{J}_n$ the approximation

$$\mathbf{J}_n \delta \mathbf{A} \approx \frac{\mathbf{F}(\mathbf{A}_n + h \delta \mathbf{A}) - \mathbf{F}(\mathbf{A}_n)}{h},$$

where h is some small number, will be used. For good preconditioning the choice of $\mathbf{F}$ is taken to be

$$\mathbf{F}(\mathbf{A}) = \mathbf{E}_{\mathbf{v}_0}^{-1} (\mathbf{b}_{\mathbf{v}(\mathbf{A})} - \mathbf{E}_{\mathbf{v}(\mathbf{A})} \mathbf{A}), \tag{15}$$

where $\mathbf{v}_0$ is the velocity field at some lower value of the Deborah number. To solve (14) using the GMRES algorithm we perform the following steps:

1. Let $\delta \mathbf{A}^{(0)}$ be an initial guess for $\delta \mathbf{A}$
2. Solve the two Stokes problems (10) and (11) with given stress fields $\mathbf{A}_n$ and $\mathbf{A}_n^* = \mathbf{A}_n + h \delta \mathbf{A}^{(0)}$
3. Compute the initial residual $\mathbf{r}_0$ from

$$\mathbf{r}_0 = -\mathbf{F}(\mathbf{A}_n) - \frac{\mathbf{F}(\mathbf{A}_n^*) - \mathbf{F}(\mathbf{A}_n)}{h}$$

At the ith iteration, an orthonormal basis $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(i)}\}$ is constructed for the Krylov subspace

$$\mathcal{K}_i(\mathbf{r}_0) \equiv \{\mathbf{r}_0, \mathbf{J}_n \mathbf{r}_0, \ldots, \mathbf{J}_n^{i-1} \mathbf{r}_0\}$$

This is usually done using a modified Gram-Schmidt procedure. However, noting the observation of Walker [29] that the modified Gram-Schmidt procedure can fail to perform well if the vectors on which it acts are not sufficiently independent, the basic GMRES code [2] has been modified by the authors so that the orthogonalization is based on the use of Householder transformations.

At the ith iteration in the GMRES algorithm a correction $\mathbf{z}_i$ is determined in $< \mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(i)} >$ which solves the least squares problem

$$\underset{\mathbf{z} \in \mathcal{K}_i(\mathbf{r}_0)}{MIN} \| - \mathbf{F} - \mathbf{J}_n(\delta \mathbf{A}^{(0)} + \mathbf{z}) \|_2 \tag{16}$$

If (16) is small enough then $\delta \mathbf{A} = \delta \mathbf{A}^{(0)} + \mathbf{z}_i$. The GMRES algorithm may thus be seen to be an inner iteration loop for every outer Newton step. Once convergence is obtained new velocity and pressure fields are computed from (10) and (11) and the procedure continued until all the variables have converged.

In both the time splitting scheme and the GMRES method the flow domain Ω is divided into several spectral elements. These are shown in Figure 2. Each of these elements is then mapped onto the parent element $D = [-1, 1] \times [-1, 1]$ using the transfinite mapping technique of Gordon and Hall [11]. The variables are approximated by finite sums of Legendre Lagrangian interpolants. The approximation spaces for the velocities and the pressure are chosen to be compatible, and there are no spurious pressure modes. The basis set for the components of stress is the same as that used for the velocities. The discrete variational problem is set up by approximating the integrals in the variational forms by Gauss-Legendre quadrature rules.

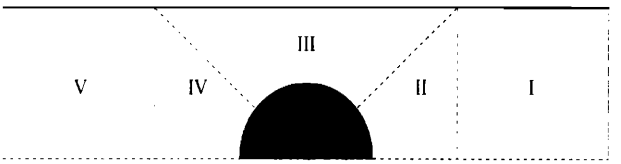

Figure 2: Domain decomposition of the flow geometry

5 Numerical results

Results for the GMRES method are presented for three different levels of discretisation ($N = 8$, $N = 12$ and $N = 14$). We consider the Oldroyd B constitutive model ($f(R) \equiv 1$). The drag on the sphere, F, is given by

$$F = -2\pi a^2 \int_0^{\pi} \{(-p + 2\eta_2 \frac{\partial u_z}{\partial z} + \tau_{zz}) \cos\theta + (\eta_2(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}) + \tau_{rz}) \sin\theta\} \sin\theta d\theta. \quad (17)$$

where the polymeric extra-stress tensor τ is given by

$$\tau = \frac{\eta_1}{\lambda_1}(\mathbf{A} - \mathbf{I}). \quad (18)$$

The drag on the sphere is determined numerically by approximating the integral in (17) using Gaussian quadrature rules. The quantity for comparison is the drag factor F^* given by

$$F^* = \frac{F}{6\pi\eta U a}$$

and is the ratio of the drag experienced by the sphere to the drag that would be experienced by the same sphere in an infinite expanse of Newtonian fluid.

5.1 Accuracy

Table 1 compares the computed drag factor F^* for modest Deborah numbers with that obtained by Lunsmann *et al* [15] who used a streamline upwinded finite element technique, and by the present authors [18] using the time splitting scheme described in section 3. The results of Lunsmann *et al* were obtained using a total of 51,354 degrees of freedom.

The finest mesh used in the calculations ($N = 14$) involves just 7595 degrees of freedom. The results from the time splitting algorithm [18] and the GMRES method with $N = 14$ show that better agreement is obtained with the results of Lunsmann *et al* for $De = 0.3$ when the GMRES method is used. Somewhat disappointing is the fact that the limiting Deborah number seemed to be about 0.6 for the $N = 8$ GMRES calculations and approximately 0.45 for higher values of N. The same sort of behaviour was observed by Fortin and Zine [10] where computations for the stick-slip problem showed that refining the mesh beyond a certain point actually resulted in a decrease in the limiting Deborah number. It is thought that the GMRES method cannot solve the ill-conditioned linear systems associated with high Deborah numbers, so that better preconditioners are called for. Discretisation errors are also responsible for numerical breakdown at the limiting Deborah numbers and there is the need to provide a better resolution of the flow field in the region near the sphere surface. A code with this capability is currently being developed by the authors. Figures 3 to 16 are contour plots produced for the flow variables using the GMRES method and computed with $N = 12$ and $De = 0.3$ and $De = 0.45$.

De	$N = 8$	$N = 12$	$N = 14$	SUFE	TSS
0.0	5.9497	5.9474	5.9474	5.9472	5.9474
0.3	5.6714	5.6946	5.6955	5.6937	5.6763
0.45	-	5.5380	5.5405	-	-
0.6	5.4471	-	-	5.4123	5.4117

Table 1: Comparison of the dependence of the drag factor on De for GMRES ($N = 8$, $N = 12$ and $N = 14$), Lunsmann *et al* (SUFE, [15]) and Owens and Phillips (TSS, $N = 14$, [18])

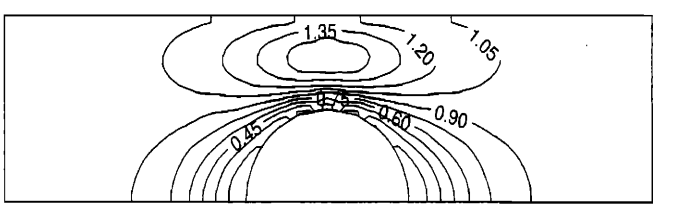

Figure 3: U_z contour plot. $De = 0.3$.

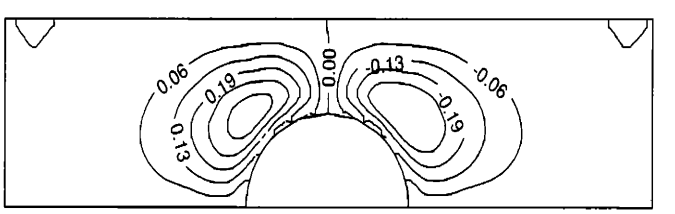

Figure 4: U_r contour plot. $De = 0.3$.

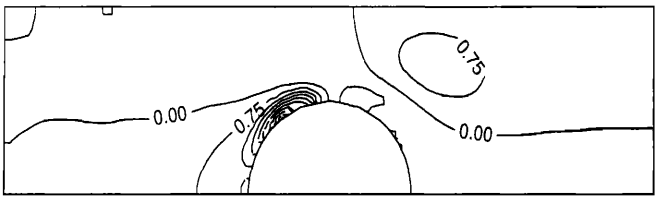

Figure 5: τ_{rr} contour plot. $De = 0.3$.

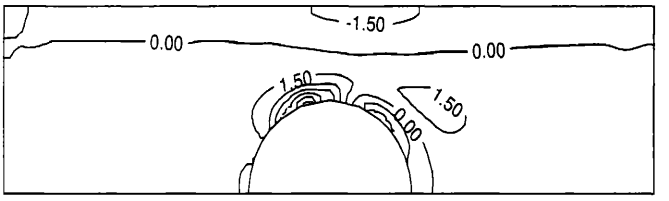

Figure 6: τ_{rz} contour plot. $De = 0.3$.

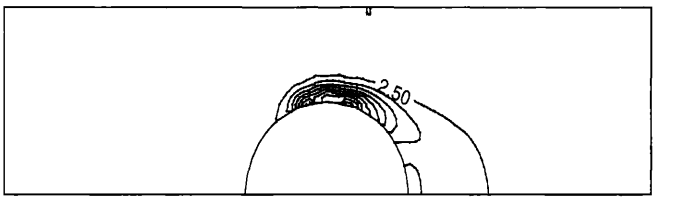

Figure 7: τ_{zz} contour plot. $De = 0.3$.

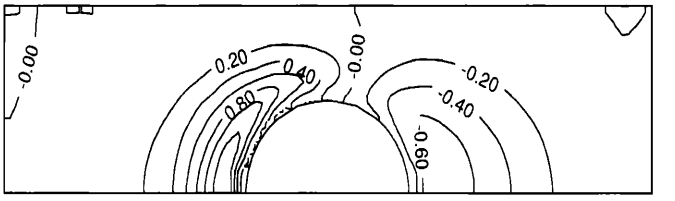

Figure 8: $\tau_{\theta\theta}$ contour plot. $De = 0.3$.

5.2 Cost

Table 2 shows the cost in CPU s on a SPARCstation 5 and number of iterations required for convergence when the two schemes were used in order to compute flow at $De = 0.3$ for $N = 4$ and $N = 6$, starting from a Newtonian flow field as the initial guess. A time step of $\Delta t = 0.01$ was used with the time stepping scheme. It may be seen that the GMRES scheme is significantly faster than the time stepping scheme, even allowing for further efficiencies which could be incorporated into the time stepping code so as to speed up the execution time. For each of the outer Newton Raphson steps (9 for $N = 4$ and 6 for $N = 6$) in the GMRES scheme, the number of inner GMRES iterations required for the residual to be less than a pre-set tolerance (in this case 1×10^{-16}) decreased monotonically after the first few Newton steps, as is to be expected. For example, for the $N = 4$ calculation the number of GMRES iterations was 37, 41, 40, 38, 37, 34, 25, 14 and 12. This makes the GMRES iterative method an efficient solver for equation (14).

N	TSS [18]	GMRES Scheme
4	721.97s, 803	126.36s, 9
6	2624.75s, 503	337.96s, 6

Table 2: Comparison of the CPU times (s) on a SPARCstation 5 and number of iterations required in simulation of viscoelastic flow at $De = 0.3$ for the two schemes.

6 Conclusions

A GMRES spectral element method has been used to compute the flow of a viscoelastic fluid past a sphere in a tube. The GMRES method is an affordable solution method for large systems of coupled nonlinear PDEs and the excessive expense of computing and inverting the full Jacobian in Newton's method has been avoided. Better agreement with the results of Lunsmann *et al* [15] has been obtained for Deborah numbers up to 0.6 when the GMRES- rather than the time splitting method is used on the same grid. The GMRES method is shown to be significantly faster than the time splitting method, although, disappointingly the limiting values of the Deborah number are modest.

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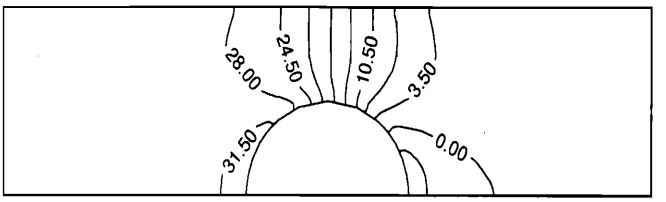

Figure 9: Pressure contour plot. $De = 0.3$.

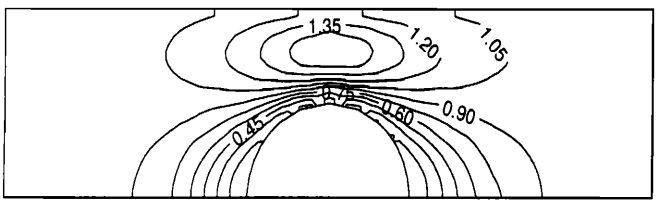

Figure 10: U_z contour plot. $De = 0.45$.

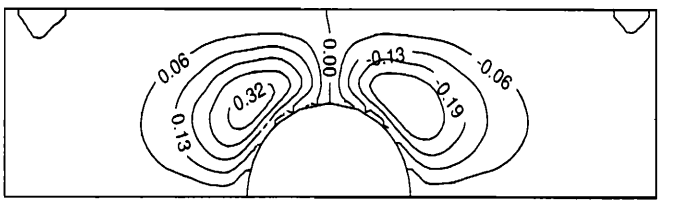

Figure 11: U_r contour plot. $De = 0.45$.

Figure 12: τ_{rr} contour plot. $De = 0.45$.

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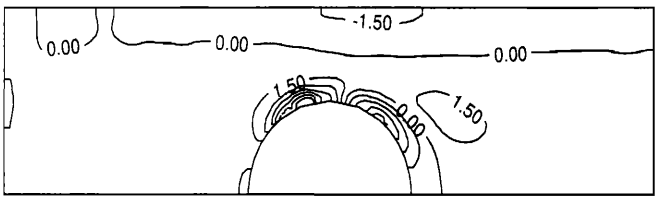

Figure 13: τ_{rz} contour plot. $De = 0.45$.

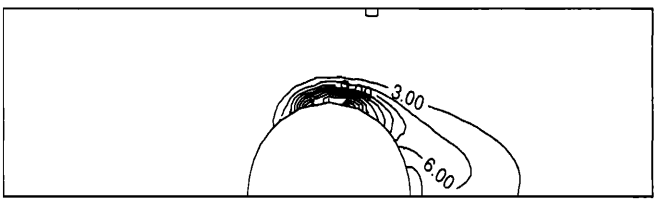

Figure 14: τ_{zz} contour plot. $De = 0.45$.

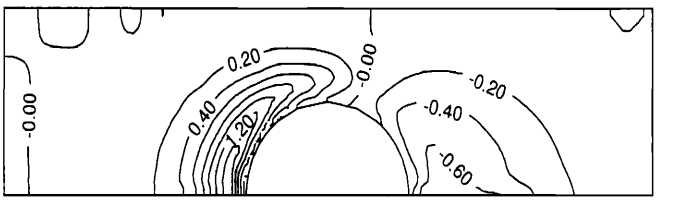

Figure 15: $\tau_{\theta\theta}$ contour plot. $De = 0.45$.

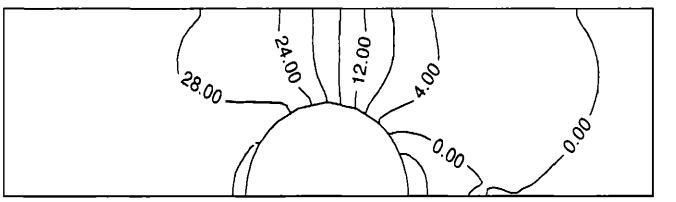

Figure 16: Pressure contour plot. $De = 0.45$.

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