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## A FAST ALGORITHM FOR NON-NEWTONIAN FLOW<sup>1</sup>

An enhanced particle-tracking finite element code for solving boundary-value problems in viscoelastic flow

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19. ABSTRACT (Continue on reverse if necessary and identify by block number) <p>This project concerned the development of a new fast finite element algorithm to solve flow problems of non-Newtonian fluids such as solutions or melts of polymers. Many constitutive theories for such materials involve single integrals over the deformation history of the particle at the stress evaluation point; examples are the Doi-Edwards and Curtiss-Bird molecular theories and the BKZ family derived from continuum arguments. These theories are believed to be among the most accurate in describing non-Newtonian effects important to polymer process design, effects such as stress relaxation, shear thinning, and normal stress effects. But the need to follow deformation histories of</p>					
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particles leads to substantial complication when flow problems are to be solved in complex geometries encountered in processing and measurement. The P. I. had developed a new algorithm that used the idea of "stream and drift function particle tracking." The purpose of the AFOSR funded research was to develop an optimized version of the algorithm which would run a factor of two faster than the pilot algorithm on scalar machines and would be able to take full advantage of vectorization on machines with that capability. The goals were achieved during the funding period. Significant progress was made in the following areas:

- code vectorization
- code enhancement and streamlining
- adaptive memory quadrature
- model problems for the High Weissenberg Number Problem
- exactly incompressible projection
- development of multimesh extrapolation procedures
- solution of problems of physical interest.

A portable version of the code is in the final stages of benchmarking and testing. It interfaces with the widely used FIDAP<sup>TM</sup> fluid dynamics package for mesh generation and post-processing, and interfaces with other pre-and post-processors can be written. The code and user's manual will be completed within a year.

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## 1. Introduction

The principal investigator developed a fast and computationally efficient implementation of a new method for the computation of steady flows of viscoelastic fluids with single-integral constitutive equations. The P. I. and coworkers had developed a new kind of finite element method to solve such problems {1} [1,2,3]<sup>2</sup>. It had been implemented, tested, and used to solve problems of physical and practical interest. The method was computationally costly, and before it could take its place as a reliable scientific and engineering tool, the P. I. believed its computational cost had to be significantly reduced, its robustness and flexibility improved, and some measure of its accuracy in benchmark problems quantified. The aim of the research was to develop an optimized algorithm that would run on the order of a factor of two faster on scalar-architecture machines than did the pilot algorithm, and would take full advantage of vectorization on machines with that capability.

During the funded research, progress was made in many areas, most prominent were: improving the efficiency of the central core of the algorithm, the stress calculator, and in a understanding of the nature of numerical difficulties which arise with some constitutive equations when the stress calculator is used to solve steady boundary-value problems. It became ever more apparent that the two issues can be separated. It is expected that that the major contribution of the completed research will have been the development of a robust and efficient stress calculator based on linear crossed triangles. Such a stress calculator has merit in its own right and can be employed with a variety of constitutive equations and with a variety of numerical schemes for the solution of the equations of steady motion of the fluid. One such scheme is the one the P. I. has been developing, which uses the crossed-triangle elements themselves to develop a pseudotime/Galerkin method. This scheme works well with some constitutive equations: Deborah numbers (non-dimensional flow rates) in excess of 25 can be achieved with a Curtiss-Bird model {1} [2--5], Deborah numbers on the order of 5 with a Wagner [5]/Johnson-Segalman {1} [5,6] fluid, on the order of 3 with an Oldroyd-B fluid [5], but only order 1 with a Maxwell fluid [5], where the "High Weissenberg Number Problem" seems most severe. A major finding of the current research is that the "particle tracking" method of the stress calculator that has been developed can also serve as the computational core of new transient

<sup>2</sup>Numbers in braces refer to the publication list of Section 8. Those in brackets refer to the Additional Reference Section 10.

algorithms for non-Newtonian flows {10} with differential constitutive relations. Implementation of these techniques and their extension to steady flows of fluids with integral constitutive equations is the subject of continuing AFOSR-sponsored research (see also Section 7., below). It is hoped that these techniques will extend the range of attainable Deborah number for those constitutive equations that currently have a limited range.

## 2. Background and Problem Formulation

The problem formulation and relevant equations are more completely described in Refs. {1} [1,2,3]; a brief summary is given here. The nondimensionalization employed here is that of Ref. {11}. The complete problem is typically to solve the following set of coupled integro-PDEs, subject to appropriate boundary and initial conditions:

$$\begin{cases} \alpha \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = \nabla \cdot \mathbf{S} \\ \mathbf{S} = -\rho \mathbf{I} + 2\varepsilon \dot{\mathbf{e}} + \boldsymbol{\tau} \\ \boldsymbol{\tau} = \int_{-\infty}^t (\mathbf{E}_t \mathbf{E}_t^T - \mathbf{I}) m(t-t') dt' \end{cases} \quad (2.1)$$

where  $\mathbf{v}$  is the velocity field,  $\mathbf{S}$  is the total (physical) stress,  $\rho$  the hydrostatic pressure,  $\dot{\mathbf{e}}$  the usual strain-rate tensor, and  $\boldsymbol{\tau}$  the non-Newtonian extra stress.  $\mathbf{E}_t$  is a strain tensor discussed in more detail shortly;  $\alpha$  is a non-dimensional ratio of Reynolds number to Deborah number, and  $\varepsilon$  is the ratio of Newtonian to polymer zero-shear viscosity {5,6,11}. The strain-dependence in the history integral in the last group of equations in Eqs. (2.1) is typical of several kinds of integral constitutive equations, for example Johnson-Segalman {1} [5,6], but the techniques described here apply to integrands with a much more complicated functional dependence on  $\mathbf{E}_t$ , such as is found, for example, in the Curtiss-Bird model {1} [2--5]. The function  $m(t-t')$  is a function of the present time,  $t$ , and historical time,  $t'$ . A typical memory function is a single exponential,

$$m(t-t') = e^{-(t-t')} \quad (2.2)$$

where, following Refs. {5,6,9,11}, it has been assumed that time has been scaled by the dominant relaxation time. Though there are many other (perhaps more physically realistic) possibilities [5], Eq. (2.2) is employed

in many currently popular models and serves as a representative example.

The key numerical difficulty addressed in the current research is the efficient and accurate evaluation of the history integral. This consists of two separate problems: first, the integrand must be evaluated, and second, the integral must be computed from sequence of such evaluations in historical time,  $t'$ . As for the first problem, the integrand is a function of the strain measured in the fluid configuration at  $t'$ , relative to the configuration at  $t$  as a reference state. This is implied by an evolution equation for the strain tensor, solved in reverse time along particle paths emanating from the stress evaluation points; a common example is given by the evolution equation associated with the 'non-affine' deformation gradient of the Johnson-Segalman model {1} [5,6],

$$\begin{cases} \dot{\mathbf{E}}_r(t') = -\mathbf{E}_r(t')(a\dot{\mathbf{e}} - \boldsymbol{\omega})(t') \\ \mathbf{E}_r(t) = \mathbf{I} \end{cases} \quad (2.3)$$

where  $\boldsymbol{\omega}$  is the spin tensor, and  $a$  is a parameter of the model; when  $a=1$  and Eq. (2.1) is used, the Maxwell model results {1} [5]. To compute particle pathlines in a time sequence of unsteady velocity fields is possible in principle, but would require the storage of a great number of velocity fields. When steady flow is assumed *a priori*, the problem is greatly simplified but still formidable. That is the focus of the current research. In the scheme described in Section 4., the time derivative in Eqs. (2.3) is retained for dynamic relaxation even when steady flow is assumed.

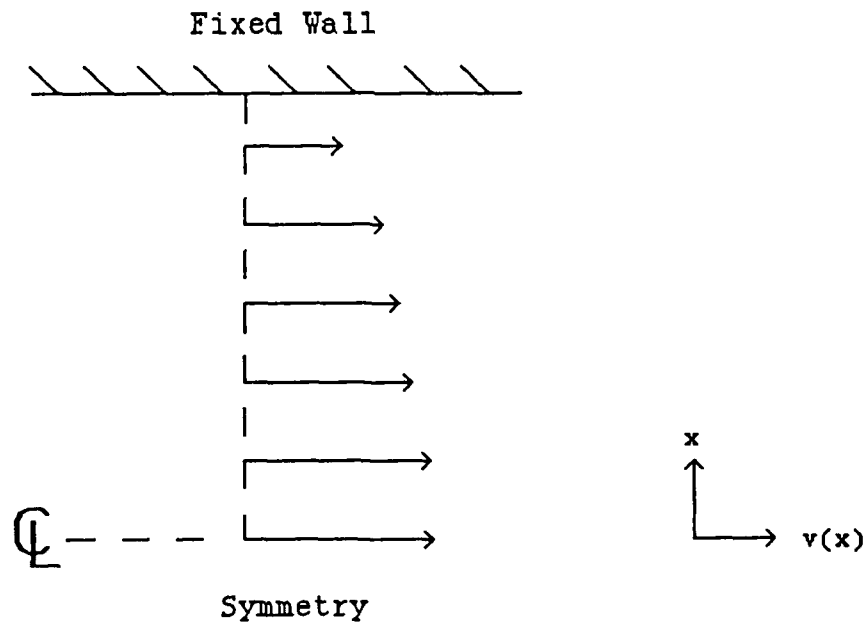
The second problem of evaluating the history integral is purely numerical and will be dealt with in Section 4.

### 3. Physical Problems

The techniques developed in the current research apply directly to isothermal, planar flow problems. The P. I.'s coworkers at Illinois Institute of Technology (see Consultative and Advisory Subsection of Interactions Section 9.) have developed methodology for extending the stress calculator techniques to axisymmetrical and non-isothermal flows [7--9]; implementation of these techniques in the Fast Algorithm is part of the P. I.'s continuing AFOSR-sponsored research. The flow problems that have been solved in the current research are idealization of flows encountered in polymer processing or property measurement. They serve as test problems that are complicated enough to fully test the techniques, but simple enough so that there is a qualitative understanding of what to

expect of the steady flow regimes.

The first problem is that of steady plane Poiseuille flow, illustrated in Fig. 3.1. This is flow between two flat, infinite plates, driven by a constant pressure gradient. The primary interest in this flow here is as boundary data for the truly two-dimensional flows. The whole question of well-posedness of planar flow problems is a delicate one and is only understood for steady flows with certain constitutive equations [10]. The P. I. has performed extensive numerical experiments and found that imposing mass conserving velocity profiles at inlets and outlets that are essentially "at infinity" works well in most cases. Further study of these matters is part of the P.I.'s NSF-sponsored research (see Support Statement Section 12.). That research also involves the study of the dynamics of shear flows leading to steady profiles such as that of Fig. 3.1 {5,6,9,11,13}. An important insight gained in that research is that the steady flow calculations described here cannot be expected to converge in certain cases because of the development of singularities in the shear rate. This matter is discussed in more detail below.



**Figure 3.1.** A plane Poiseuille flow profile. This flow is used as boundary data in some of the planar flows. Symmetry is assumed in this figure, but the full profile is also useful as boundary data in cases where enforced symmetry is not appropriate.

Fig. 3.2 illustrates planar contraction flow. The pictured domain is a cross-section of a wide channel with an abrupt change in height; only the upper half of the channel is modelled because symmetry of the geometry

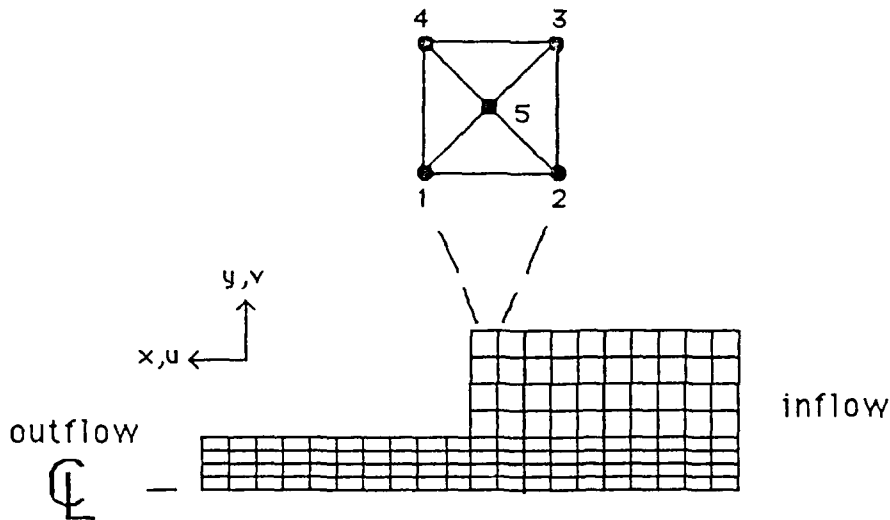
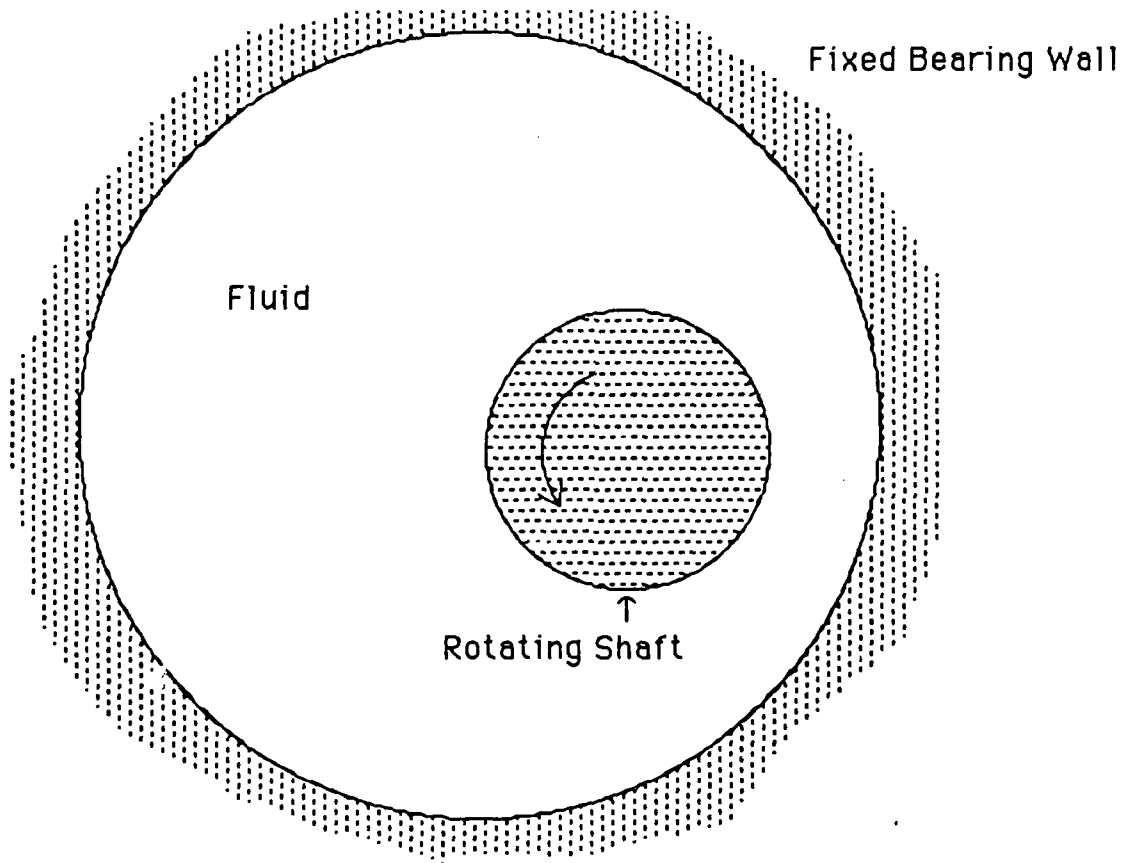


Figure 3.2. Abrupt contraction flow test problem, showing a very crude mesh. Inflows and outflows are assumed to be far enough from the region of disturbed flow so that plane Poiseuille flow can be imposed (see Fig. 3.1). The inset shows a square special case of the quadrilateral crossed triangle macroelement used in this research; it is composed of four constant strain-rate triangles formed by crossing quadrilateral diagonals.

and resulting flow is assumed. A major reason for studying the abrupt contraction flow is that the singularity in shear rate induced by the corner appears to be significant, though its order is not known for most non-Newtonian fluids [1].

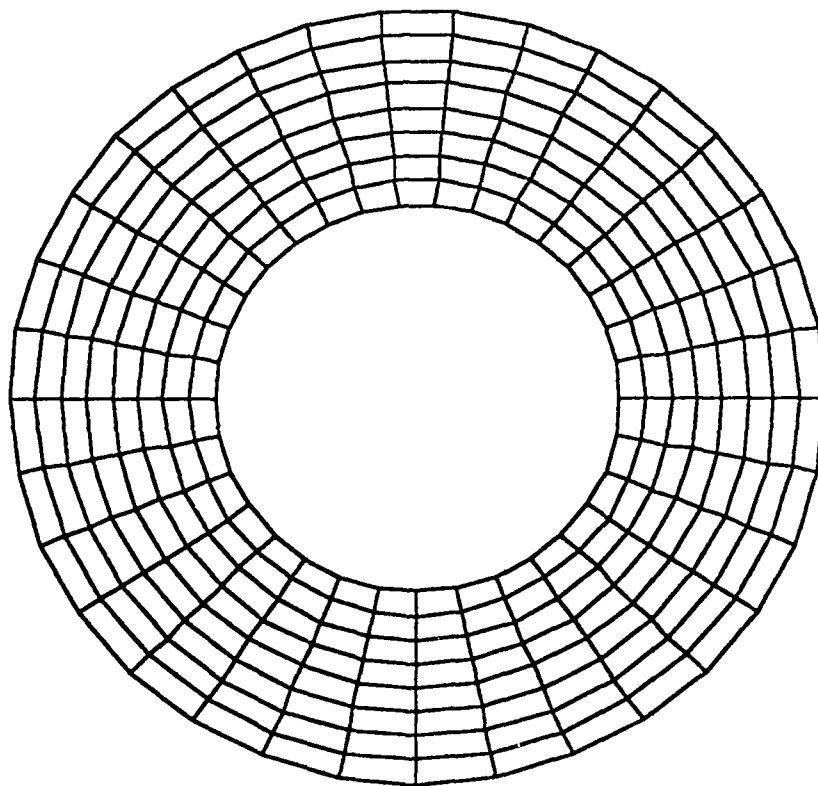
The journal bearing problem illustrated in Fig. 3.3 is an idealization of an important lubrication flow. In most actual lubrication applications (main bearings in internal combustion engines, for example), the lubricating film is so thin that the gap between bearing and shaft is too narrow to be modelled by the techniques described here; however, the eccentric geometry is of interest, because for larger gaps it provides a problem for which spectral techniques can provide accurate numerical solutions at very high Deborah number [11]. These solutions can be used as benchmarks for fully discrete methods; this has led others to develop new numerical formulations for differential constitutive equations that are

very successful at high Deborah number [12]. It is hoped that similar benefits to integral formulations will accrue in the future. One of the most important points about the journal bearing problem is that there are no corners in the domain and no inflows or outflows. The concentric case 'true Couette flow' is of interest because the exact solution is known.



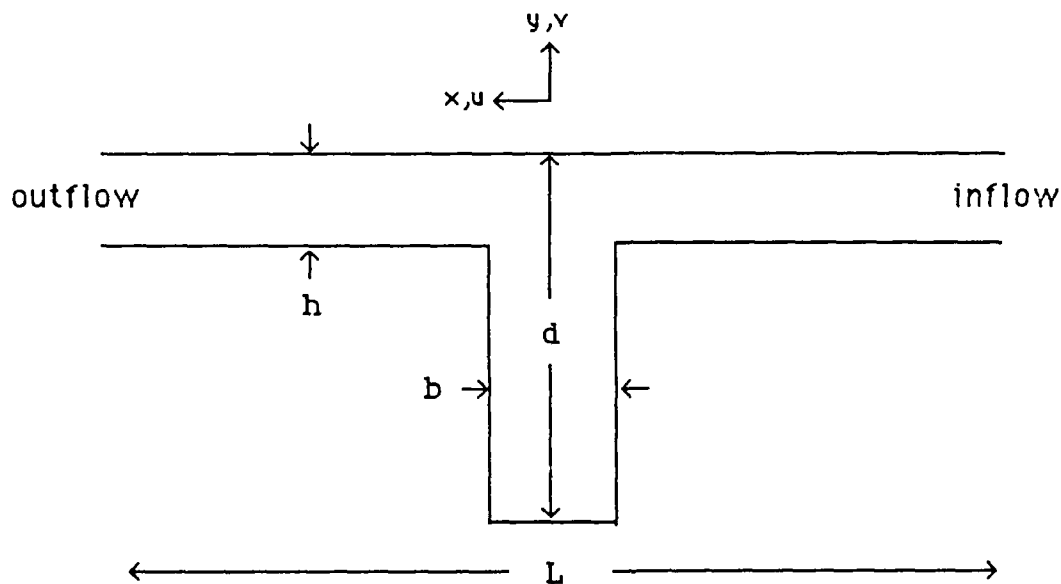
**Figure 3.3.** Domain for journal bearing problem. This highly idealized approximation to a lubrication flow is a standard test problem in which a wide variety of gaps and eccentricities can be specified. The most numerical difficulty occurs for high eccentricity and narrow gaps.

Because the eccentric cylinder geometry is of such mathematical and numerical interest, experimenters have been led to make flow visualization apparatus incorporating this geometry [13], and the P. I. has extensive Laser Doppler Velocimetry data for such flows at his disposal. Making a comparison between computed and observed solutions is an important component of the P. I.'s continuing AFOSR-sponsored research.



**Figure 3.4.** Mesh for journal bearing problem in special case when shaft and bearing are concentric; exact solution is known for this test problem. For the crossed triangle macroelement of Fig. 3.2, using an odd number of elements in each circumferential strip is essential to avoid 'checkerboard' problems.

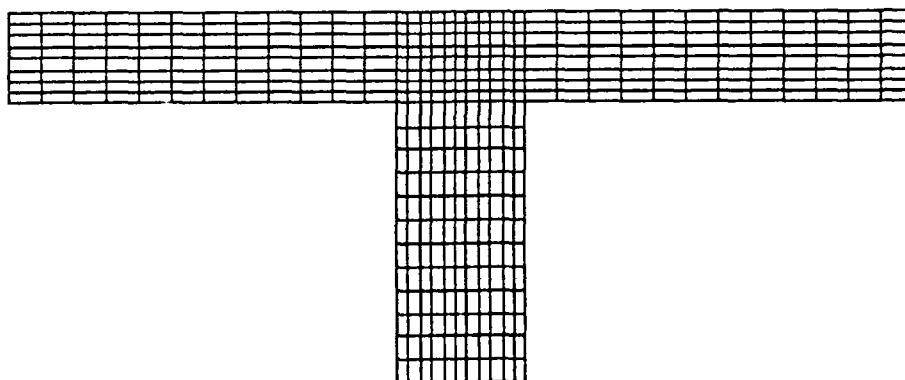
The problem to which most effort in the current research has been devoted is that of a plane flow over a transverse slot, pictured in Fig. 3.5. If the pictured flow is driven by motion of the upper plate, we say the flow has "Couette base flow"; if it is driven by an applied pressure gradient while both walls stay fixed, we say that it has "(plane) Poiseuille base flow." This flow (with Poiseuille base flow) is the basis of a unique in-line measurement device for measuring viscosity and first normal stress differences of polymer solutions and melts, the Lodge Stressmeter™ {1,2,8,12} [2,3,5,14]. The device uses the 'elastic hole pressure' [2,3,14] to predict the first normal stress difference. The elastic hole pressure is the difference in thrust between the top



**Figure 3.5.** Domain for slot flow problem;  $h$ ,  $b$ , and  $d$  are physical dimensions that correspond to actual device parameters.  $L$  is assumed to be large enough so that plane Poiseuille flow can be imposed at the in-and outflows to a reasonable degree of accuracy (see Fig. 3.1).

and bottom of the slot, minus the inertial contribution to the hole pressure [2,3,14]. The shear viscosity is measured by a rather straightforward estimation of the pressure gradient [14] [In fact, actual devices have two widely separated slots for this purpose.], but the normal stress measurement is based on a rather subtle measurement

relation [15]. A major reason for studying this flow is the "Higashitani-Pritchard-Baird-Lodge (HPBL) Paradox": The derivation of the HPBL measurement relation in Ref. [15] can only be approximately correct in Couette base flow [17]; in the Poiseuille base flow, the derivation leaves out terms that are  $O(1)$  with respect to the measured quantities [12] [16], yet the measurement relation appears to be correct. This paradox was uncovered by the P. I. and his Research Assistant during the funding period (and independently by R. Srinivasan [16]); it now appears to be resolved (as outlined in the Status of Research Section 5.). This aspect of the problem is a major component of the thesis work described in the Publications Section 8 (Ref. [17]).

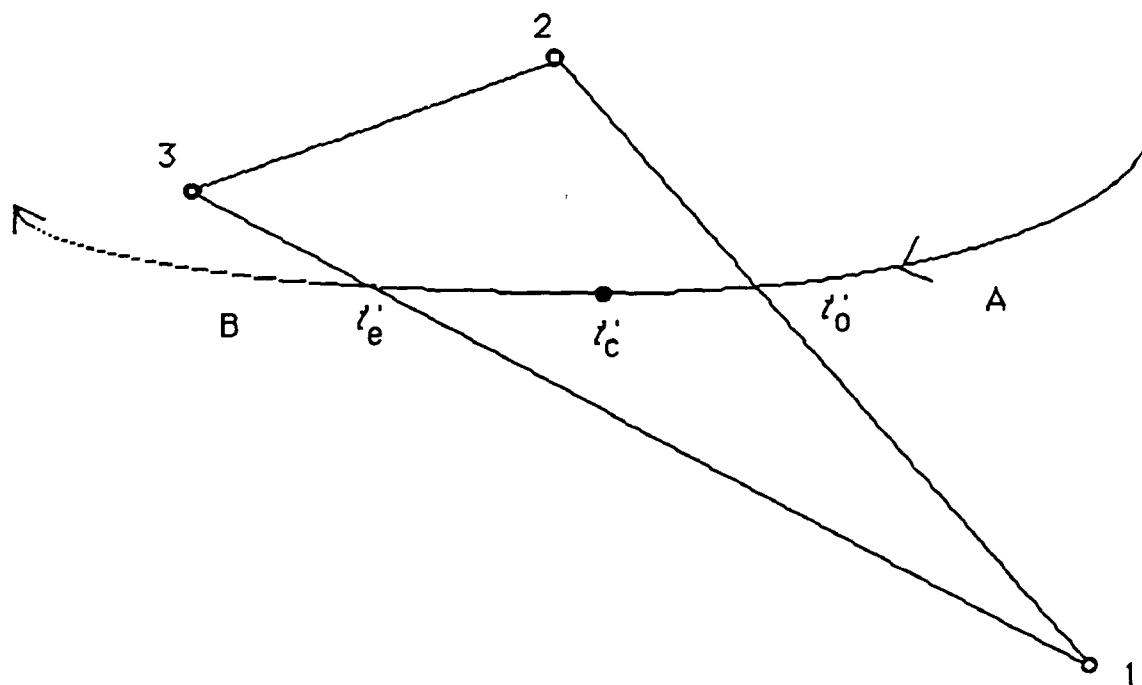


**Figure 3.6.** Typical mesh for slot flow problem. Grid is finest in the slot mouth area, where experience shows that the curvature of the streamlines in the channel and at the top of the vortex in the slot are crucial to accurate determination of the hole pressure.

During the funding period other aspects of slot flow have been studied, particularly the excess pressure rise in the base Couette or Poiseuille flow due to the slot disturbance. The slot flow problem is also interesting for the qualitative features observed. One such feature is the appearance of vortices in the slot itself; these have been the subject of extensive flow visualization study [17].

#### 4. Tools and Techniques

Equations (2.1) are solved by a standard Galerkin formulation, based on the crossed triangle macroelement illustrated in Fig. 3.2 [1,2,3]. The history integral is evaluated by a weighted quadrature formula that includes the memory function in the weights. When the memory function is the single exponential of Eq. (2.2), the quadrature formula is a Laguerre formula, otherwise it is some appropriate generalization of a Laguerre formula [2]. To evaluate the integrand of the history integral of Eqs. (2.1)



**Figure 4.1.** A constant strain-rate triangle showing a conic section streamline/particle path. Arrows indicate flow direction. Filled circle is the location of the centroid/stress evaluation point in the first element and the location at which the generalized Laguerre point is found in succeeding elements (not necessarily the centroid);  $t'_c$  is 0 for the stress evaluation element and is a generalized Laguerre time otherwise;  $t'_e$  and  $t'_o$  are element boundary crossing times.

"particle tracking" is used. This technique is described in detail in [1,2,3], and is illustrated in Fig. 4.1. Tracking is performed from centroid of triangle where stress is evaluated with historical time  $t'_c=0$ , following path A backwards along the upstream portion of the streamline, emanating

from the centroid at the filled circle. In succeeding elements the paths are like the union of portions A and B, with boundary crossing times  $t'_e$  and  $t'_o$ . This tracking is continued back into the past until such time as a temporal generalized Laguerre point is reached at time  $t'_c$  at the spatial location of the filled circle (now not necessarily the element centroid). The integrand is evaluated, and the process continues until the last integration point is encountered.

The crossed triangle macroelement is ideally suited to this procedure because it has excellent mass conservation properties and constant velocity gradients on each triangle [2,3]. In this case, one finds that Eqs. (2.3) have an exact solution on each triangle, at any historical time  $t'$  between  $t'_o$  and  $t'_e$ . This solution is given by

$$\mathbf{E}_i(t') = (\cosh[\delta(t' - t'_o)])\mathbf{E}_i(t'_o) - \frac{\sinh[\delta(t' - t'_o)]}{\delta}\mathbf{E}_i(t'_o)\mathbf{A} \quad (4.1)$$

where  $\mathbf{A}$  is the coefficient matrix in Eqs. (2.3) and  $\delta$  is its eigenvalue (with a plus sign). Using the initial condition of Eqs. (2.3) and accumulating the strain multiplicatively according to Eq. (4.1), the integrand can be calculated analytically along the streamline. Two essential features of these calculations are [2,3]: 1) The streamlines are conic sections on each element and  $C_1$  at element boundaries, and 2) there is an analytic relation between any two points  $\mathbf{x}_1$  and  $\mathbf{x}_2$  on a streamline and the transit time between these points, given by the drift function,

$$t'_1 - t'_2 = w(\mathbf{x}_1) - w(\mathbf{x}_2) \quad (4.2)$$

The calculations just described allow evaluation of the history integral, thus the total stress at any triangle centroid in the domain. This procedure is embedded in an implicit-explicit pseudotime/Galerkin scheme, generalizing that of Hughes, Liu, and Brooks [18]. In the following equations, the time level is denoted by subscripts  $n$  or  $n+1$  and inner iterations by superscripts  $(0)$ ,  $(i)$ , or  $(i+1)$ . Absence of superscripts indicates fully converged inner iteration.

$$\left\{ \begin{array}{l}
\mathbf{M}\mathbf{a}_{n+1} + \mathbf{C}\mathbf{v}_{n+1} + \mathbf{P}(\mathbf{v}_{n+1}) + \mathbf{Q}(\mathbf{v}_{n+1}) = \mathbf{F}_{n+1} \\
\mathbf{P}(\mathbf{v}) = \alpha \int_{\Omega} \mathbf{N}^T (\mathbf{v} \cdot \nabla \mathbf{v}) dV \\
\mathbf{Q}(\mathbf{v}) = \int_{\Omega} \mathbf{B}^T \mathbf{S} dV - \mathbf{C}\mathbf{v} \\
\mathbf{v}_{n+1}^{(0)} = \mathbf{v}_n + (1 - \gamma) \Delta t \mathbf{a}_n \\
\mathbf{v}_{n+1}^{(i+1)} = \mathbf{v}_{n+1}^{(i)} - \mathbf{J}^{-1} \left\{ [\mathbf{M} + \gamma \Delta t \mathbf{C}] \mathbf{v}_{n+1}^{(i)} + \gamma \Delta t \mathbf{Q}(\mathbf{v}_{n+1}^{(i)}) \right. \\
\quad \left. + \gamma \Delta t \mathbf{P}(\mathbf{v}_{n+1}^{(i)}) - \mathbf{M}\mathbf{v}_{n+1}^{(0)} + \gamma \Delta t \mathbf{F}_{n+1} \right\} \\
\mathbf{a}_{n+1} = (\mathbf{v}_{n+1} - \mathbf{v}_{n+1}^{(0)}) / \gamma \Delta t \\
\mathbf{J} = \mathbf{M} + \gamma \Delta t \mathbf{C} + \left( \gamma \Delta t \frac{\partial \mathbf{P}}{\partial \mathbf{v}} \right)_{opt} + \left( \gamma \Delta t \frac{\partial \mathbf{Q}}{\partial \mathbf{v}} \right)_{opt}
\end{array} \right. \quad (4.3)$$

**M** and **C** are the usual finite element mass and dissipation/penalty {1,2,3} matrices, corresponding to the nondimensionalization of Eqs. (2.1) or in analogous dimensional form. **P** is the nonlinear contribution to the material derivative, and **Q(v)** is the non-Newtonian contribution to the total stress, with **S** computed from the indicated velocity field by particle tracking. **N** is the matrix of shape functions and **B** the usual finite element 'B-matrix' {18}. **J** is an approximation to the Jacobian of the residual expression in the braces following its inverse, and  $\gamma$  is parameter of the integration scheme usually chosen to be between 0.5 and 1. The 'opt' subscripts on the second two terms in the definition of **J** indicate that this Jacobian information is optional. In the current algorithm these terms are omitted, in order to preserve symmetry and simplicity of the matrices involved. Two compensatory techniques are employed: 1) An inverse Broyden quasi-Newton scheme is used that has the effect of approximating these terms as the inner iterations proceed, and 2) an unwinding scheme generalizing that of Ref. [18] to constant strain-rate triangles is used on the inertial terms. Though the unwinding scheme is not particularly sophisticated, it seems to work very well at the lower Reynolds numbers characteristic of the very viscous flows studied in this research.

When  $\mathbf{Q} \neq 0$ , the integration scheme of Eqs. (4.3) is a 'pseudotime scheme' because, though the time derivative in the inertial term is retained and differenced, the time-dependence of **Q** is not properly taken into account. The stress is calculated assuming that the current velocity field takes the place of all velocity fields in the past, so that these need not be stored. This assumption is only valid when steady flow is

to the steady state. This feature must be viewed as a limitation of the approach, but the alternative of fully dynamic simulation with integral models seems out of reach at present. The hope is that the algorithmic damping of the pseudotime scheme will lead to a more rapid convergence at higher Deborah numbers than can be achieved with direct steady iteration. It should be noted that direct steady iteration can be obtained from Eqs. (4.3) as  $\Delta t \rightarrow \infty$  by taking  $\gamma=1$ .

The key issue in the algorithm of Eqs. (4.3) is the efficient evaluation of the extra stress, for each of many inner iterates. This is a computationally burdensome calculation, since many generalized Laguerre points are required to obtain accurate stresses; this implies that thousands of element-level tracking calculations must be carried out for each iteration.

## 5. Status of the Research

During the reporting period, research progress has been made in several areas:

1. Vectorization of the fast algorithm: The vectorization of the P. I.'s code for two supercomputers has been completed, and the P. I. and his Research Assistant are in the process of preparing a version of the code for the SDSC Cray XMP/48. The resulting improvements are detailed in Section 6. As expected, since particle tracking involves so many element level calculations, vectorization did not make as much a relative difference for non-Newtonian flow as it did for Newtonian (Navier-Stokes) flow. Other enhancements described in the next subsection proved to be more effective in the non-Newtonian case.
2. Code enhancement and streamlining: In current supercomputing environments core storage capacity is enormous with respect to the needs of the P. I.'s code; this is also true in virtual memory environments. It has proved extremely cost-effective to avoid regeneration of element-level quantities wherever possible, in favor of arrays that are permanent or redefined only at the outset of each iteration. Unlike standard finite element procedures, those for memory fluids must repeatedly use information which is nonlinearly dependent on the current the velocity field at the current time step. For standard finite element procedures, the choice is to generate the information as needed, discarding the result after it is used. Here, it

pays to generate element data such as strain rate and save it in a large array at the outset of each inner iteration at each pseudotime step. Since each element can contain the pathlines of many material points required to compute the new stress field, numerous regenerations of the data from nodal values can be avoided. For the P. I. 's code the saving attributable to this trade-off was found to be 20% to compute a solution in abrupt contraction flow for a Johnson-Segalman/Wagner fluid at Deborah number 5.

3. Adaptive memory quadrature: This is the technique of determining the number of generalized Laguerre points for each triangle, based on the maximum shear-rate encountered on the particle path emanating from the element in the previous iteration. A simple thresholding scheme was used in which all triangles with relatively high shear rates use the maximum available number of quadrature points, but triangles with significantly lower shear rates use a reduced number. It has been found that a substantial reduction in running time can be obtained with the Maxwell fluid model from the adaptive quadrature alone. The saving is less for more complicated constitutive equations but still is significant. For the Johnson-Segalman/Wagner fluid in abrupt contraction flow at Deborah number 5, the saving due to adaptive quadrature was found to be about 20%. Note that the combined savings of items 2. and 3. amount to a reduction of 40% in CPU cost in the Johnson-Segalman/Wagner case and much more in the Maxwell fluid case.
  
4. Model problems for the High Weissenberg Number Problem (HWNP): This term refers to the pathologies which cause difficulty in converging to solutions with significant non-Newtonian effects when many constitutive equations are employed [1]. The P. I. has succeeded in developing a simple, analytically tractable model which shows possible sources of the HWNP [13]. In the model problem, the combined equations of steady motion and stress lose their ellipticity with increasing flow rate. This can be treated in 1-D by techniques that are closely related to optimal upwinding techniques for the Navier-Stokes equations. In two space dimensions the problem is more difficult: Added viscosity *must* be anisotropic; previous attempts to add 'Newtonian' viscosity seem to have failed for this reason. It is also unclear how to define a

'Peclet-like' number for planar flows; anisotropy indicates that there should be at least two of them.

Further attempts to extend the concept of anisotropic viscosity were deferred because of two interesting discoveries: First, in the analysis of the equations of motion and stress for a Johnson-Segalman model with a very small amount of 'Newtonian viscosity,' it was found that the full system had an unsteady transition to asymptotically steady 'spurt' solutions with 'singular surfaces' {5,6,9,11,14} [19]. These solutions are believed to be physically important and can be related to the phenomenon of 'melt fracture' [20]. The added viscosity techniques would artificially suppress such phenomena, because their signature is precisely the loss of ellipticity in the steady equations. Second, for spurt solutions in shear-flow, numerical methods suggested themselves which require no anisotropic viscosity, which are fully dynamic, and are robust to the development of singular surfaces. The extension of these methods to 2-D flows is the central focus of this continuing AFOSR-sponsored research. The key insight is that the loss of ellipticity of the steady equations is only fatal to methods which 'parabolize' the steady flow problem, either by direct stationary iteration --- which is analogous to a pseudotime scheme for *parabolic equations* --- or by the overt introduction of such a pseudotime. Ellipticity loss is not fatal to schemes which respect hyperbolic character, and the P. I. proposes that the new, efficient stress calculator can be imbedded in such schemes.

5. Exactly incompressible projection: This is a technique for the removal of residual compressibility from finite element interpolations to velocity fields. It was developed by E. T. Olsen (Dept. Mathematics, I.I.T.) as part of the P. I.'s joint research with the I.I.T. group (see 'Interactions' Section 9. following). The idea is to project the slightly compressible field onto the weakly incompressible fields (which, for the crossed triangle element, are exactly incompressible) in some convenient norm. The normal equations are solved by conjugate-gradients without assembly of the system matrix. Since the correction is typically very small, the process is rapidly convergent. The need for projection arises from the fact that the 'tracking' procedure assumes exact incompressibility. When the slight compressibility arises from the penalty used to give pressure approximations, it is negligible for

the purpose of tracking, except in some extreme and rarely occurring cases. But when the stress calculator is used on experimentally observed velocity fields, experimental and interpolation error could lead to significant artificial compressibility which must be eliminated before the stress calculator can function reliably.

6. Development of multimesh extrapolation procedures: In the early phases of the current research, the P. I. was puzzled by the fact that numerical solutions failed to confirm the HPBL measurement relation (see Section 3.) [2,3,5]. M. F. Webster (formerly Reading, U. K., now University College, Swansea) reported good agreement between finite difference solutions and the HPBL relation. At the P. I.'s encouraging, Webster performed grid refinement studies and found that the results changed and there was poorer agreement with the HPBL relation on finer grids. The P. I. and Webster collaborated in the development of Richardson extrapolation techniques to investigate the behavior of our respective numerical schemes [2]. We found that for the Maxwell model, for which both of our numerical methods could be used, exhibits slow first order convergence of the modelled slot pressure, using the P. I.'s finite element method, and non-monotonic second-order convergence for the finite difference scheme. Both methods appeared to be converging to the same hole pressures and related quantities, but would require very fine grids to get produce hole pressures in line with the HPBL predictions; however, the extrapolated results agreed well between the two methods and gave good agreement with the HPBL relation. Agreement with the HPBL relation for the Maxwell fluid in planar slot flow was later confirmed by Sugeng, Phan-Thien, and Tanner [21], using a boundary element method. With some other constitutive equations, such as Curtiss-Bird [4], in which disagreement with the HPBL relation is observed, the error indicators developed in conjunction with the extrapolation techniques yield ambiguous results, and their satisfaction of the HPBL relation is still an open question.

7. The solution of problems of physical interest: In spite of the Deborah number limitations of the current pseudotime approach, significant progress was made in the understanding of several interesting problems. In flows over transverse slots it was discovered that, while the HPBL measurement relation is apparently misapplied to pressure-

gradient driven flows, its predictions are evidently correct. The thesis work of M. Yao [17] shows promise of explaining this paradox. We find that the derivation of the HPBL relation contains two steps that are only approximately correct; with a Couette base flow, for a Maxwell or Oldroyd-B [5] fluid, the approximations are accurate, but with plane Poiseuille base flow they are not; however the error from the two questionable steps cancels, leading to a correct result. Mr. Yao is continuing to investigate the possibility of error cancellation with other constitutive equations. One of the approximate steps in the HPBL analysis is the dropping of the streamwise gradient of the normal stress. One might suppose that this is a reasonable assumption with Couette base flow, but we have found that there can be a significant pressure rise in such flows, induced by the disturbance of the slot. Fortunately, in the derivation of the HPBL relation, the integral contribution from this pressure rise is small with Couette base flow. We have studied these slot-induced pressure rises with both Couette and Poiseuille base flows, and details of the investigation will be found Ref. [17]. We have also computed flows in abrupt contraction

	<b>Slot Flow</b>		<b>Contraction Flow</b>		<b>Journal Bearing</b>	
	<b><u>Maxwell Stress C.</u></b>		<b><u>Maxwell Stress C.</u></b>		<b><u>Maxwell Stress C.</u></b>	
<b>De</b>	0.9167	3.3040	1.3290	4.7520	4.4165	8.8500
<b>Iters.</b>	7	12	9	8	4	10
<b>CPU</b>	230	394	174	207	123	700

**Table 5.1** Summary of maximum Deborah number ( $De$ ) and CPU time in minutes achieved by the pseudotime/Galerkin method in various flows. 'Stress C.' refers to a single integral model with similar characteristics to a modified Phan-Thien/Tanner model [5]. Slightly higher  $De$  can probably be achieved in slot flow. Deborah numbers in excess of 25 can be achieved with this method using the Curtiss-Bird [4] constitutive equation, but the new, fast stress calculator has not been implemented to use that constitutive equation yet. The mesh for slot flow has 1008 macroelements [2], for contraction flow 940, and for journal bearing flow 384 macros. CPU times are for a VAX 11/780 using double precision arithmetic.

and in planar idealizations of journal bearings. In the latter case, we are involved in a detailed comparison of our results with experimental velocity measurements (the thesis work of S. Burdette [13]). Table 1 gives a summary of the maximum Deborah numbers achieved and the

computational cost on a Vax 11/780. A more complete description of these results and others will be found in Ref. {17}.

## 6. Performance Improvement

The central focus of the funded research was to improve the performance of the original pilot code and enhance its usefulness as a research tool. The following summary is excerpted from Ref. {17}. The pilot code referred to as FLUCODE Version 0.0 had already been modified and enhanced by the P. I. under the current project (for example, a preliminary version of adaptive memory quadrature had been implemented) and thus represents a more advanced version of the code than the original pilot version. The performance improvement documented below in addition to the enhancements already made in Version 0.0 add up to an average performance improvement in excess of the project target of a factor of two improvement in running time. For example, in the preparation of Ref. {2}, a run comparable to Column 1 of Table 5.1 was made with the basic pilot code. It required 16 iterations and 677 CPU minutes. According to Table 5.1, the enhanced algorithm has reduced the number of required iterations by more than a factor of two and reduced the CPU time per iteration by 22% over the basic pilot version.

Mr. Yao has also developed an interface with FIDAP [22] for pre-and postprocessing. This fluid dynamics analysis package is widely used and makes FLUCODE more easily accessible to other researchers. It is interesting to note that FLUCODE and FIDAP can both solve Navier-Stokes problems, and that the Navier-Stokes solver in FLUCODE performs very well in comparison to FIDAP. It should be pointed out, however, that FIDAP has many general purpose features that FLUCODE does not.

The versions of FLUCODE are designated as follows:

- Version 0.0 - pilot code developed by D.S. Malkus, *et al.*
- Version 0.1 - vectorized code of version 0.0;
- Version 1.0 - the earlier stage of the new version (modified by M. Yao) without storing the geometrical, material and iterational quantities;
- Version 1.1 - the newest VAX version of FLUCODE (modified by M. Yao);
- Version 1.2 the newest CRAY-2 version of FLUCODE (modified by M. Yao).

The test problem referred in this section is the *4:1 Abrupt Contraction Flow Simulation* of Fig. 3.2, described in Section 3. The symmetry of flow

domain is assumed and three cases are considered:

- Stokes solution,  $Re=0$ , linear case;
- Navier-Stokes solution,  $Re=80$ , 56 explicit time steps,  $\Delta t=0.02$ ;
- Modified Johnson-Segalman fluid,  $De=0.3$ ,
  - \*pseudotime step with predictor-corrector plus 1 inner iteration,  $\Delta t=1.0$ ,
  - \*explicit pseudotime steps,  $\Delta t=1.0$ .

Significant performance improvement has been achieved by the newest version of FLUCODE. Table 6.1 shows the performance improvement on the VAX 11/780 and performance comparison with FIDAP, for the Stokes solution case. The improvement of Version 1.1 is about 21% over Version 0.0. The performance improvement for the Navier-Stokes solution case can be seen in Table 6.2 & 6.3. There is about 25% CPU saving for the Navier-Stokes solution for Version 1.1 on the VAX. Tables 6.4 to Table 6.6 show the modified Johnson-Segalman fluid case. From Table 3.5 we can see that the performance improvement of version 1.2 on the CRAY-2 is about 34% over Version 0.1. This is, in some part, due to storing the geometrical and material information at the beginning and the intermediate iteration information at each time step instead of re-calculating them. As a price, the in-core storage needed in the newest version is much larger than Version 0.0.

<u>CODE</u>	<u>CPU (seconds)</u>
FLUCODE 0.0	135.8
FLUCODE 1.0	110.5
FLUCODE 1.1	107.0
FIDAP 2.0	226.3

Table 6.1 Performance Improvement on VAX-11/780  
4:1 Abrupt Contraction Flow (940 elements, 1024  
nodes) Stokes Solution ( $Re=0$ ).

<u>CODE</u>	<u>Iterations</u>	<u>CPU(sec.)</u>
FLUCODE 0.0	56	1646.3
FLUCODE 1.1	56	1239.1
FLUCODE 1.1	1	197.0
FIDAP 2.0	1	373.0

Table 6.2 Performance Improvement on VAX 11/780  
4:1 Abrupt Contraction Flow (940 elements, 1024  
nodes) Navier-Stokes Solution ( $Re=80$ ).

### CRAY-2 at U. of Minnesota

<u>FLUCODE</u>	<u>Compiler</u>	<u>Vector</u>	<u>Iters.</u>	<u>CPU(sec.)</u>
0.0	cft77 0.23	disabled	56	81
0.1	cft77 0.23	disabled	56	79
0.1	cft77 0.23	enabled	56	57
1.2	cft77 1.3a	enabled	56	--

Table 6.3 Performance Improvement on CRAY-2 4:1 Abrupt  
Contraction Flow (940 elements, 1024 nodes ) Navier-Stokes  
Solution ( $Re=80$ ).

### VAX-11/780 at CMS -- U. of Wisconsin

<u>FLUCODE</u>	<u>Compiler</u>	<u>Iterations</u>	<u>CPU(sec.)</u>
0.0	Fortran	1	2881
1.0	Fortran	1	2407
1.1	Fortran	1	----
0.0	Fortran	3	4862
1.0	Fortran	3	3906
1.1	Fortran	3	3348

Table 6.4 Performance Improvement on VAX-11/780 4:1  
Abrupt Contraction Flow (940 elements, 1024 nodes) Modified  
Johnson-Segalman fluids with  $De \approx 0.3$ .

### CRAY-2 at U. of Minnesota

<u>FLUCODE</u>	<u>Compiler</u>	<u>Uector</u>	<u>Iters.</u>	<u>CPU(sec.)</u>
0.0	cft77 0.23	disabled	3	158
0.1	cft77 0.23	disabled	3	157
0.1	cft77 0.23	enabled	3	139
1.2	cft77 1.3a	enabled	3	92

Table 6.5 Performance Improvement on CRAY-2 4:1 Abrupt Contraction Flow (940 elements, 1024 nodes) Modified Johnson-Segalman fluids with  $De=0.3$ .

### CYBER-205 at U. of Minnesota

<u>FLUCODE</u>	<u>De</u>	<u>Compiler</u>	<u>Uector</u>	<u>Iters.</u>	<u>CPU(sec.)</u>
0.0	0.3	ftn 200	disabled	3	487
0.1	0.3	VAST ftn	enabled	3	328
0.0	3.0	VAST ftn	enabled	--	721

Table 6.6 Performance on CYBER-205 4:1 Abrupt Contraction Flow (940 elements, 1024 nodes) Modified Johnson-Segalman fluids.

## 7. Conclusions and Future Directions

The following positive conclusions may be drawn from the completed research:

- The pilot algorithm has been significantly enhanced and improved during the funding period.
- In a modern computing environment, particle tracking stress calculations can be performed at reasonable cost on realistic grids.
- The new algorithm has been used to gain physical insight in several important flow problems relevant to polymer processing and measurement.

- Continuing investigation of physical problems for which experimental results exist promises to shed further light on the modelling of polymeric systems.
- The stress calculator can operate independently of the pseudotime/Galerkin method to calculate non-Newtonian extra stresses from experimentally determined velocity fields or to be embedded in other solution schemes for the equations of motion.

On the other hand, the techniques developed to date are subject to the following limitations:

- The techniques are limited to planar and (in the future) axisymmetric flows.
- Flows that develop singularities as time evolves seem to be inaccessible to the pseudotime/Galerkin method for single integral constitutive equations.
- Transient analysis using integral models seems prohibitively expensive in the current computing environment.

However, a major finding of the completed research is:

- The particle tracking technique can be the core of fully dynamic methods for differential models that show promise of being robust to the development of singularities.

This last point is the focus of continuing AFOSR-sponsored research. A preliminary description of the use of the stress calculator for differential models can be found in Ref. {10}. The fundamental idea is to extend the techniques for dynamic shear flows {5,6,9,11,14} to planar flows by replacing the convected derivatives with a 'Lagrangian difference quotient' along streamlines. This combines Galerkin finite element techniques with a 'method of characteristics' solution for the stress.

## 8. Publications

### *Journal and Reviewed Proceeding Articles Appearing or Accepted During Reporting Period*

1. D. S. Malkus, "Finite element methods for viscoelastic flow," *Viscoelasticity and Rheology (Madison, 1985)*, Proceedings of Mathematics Research Center Symposium, October 1984, A. S. Lodge, J. A. Nohel and M. Renardy, co-editors, Academic Press, Inc., New York (1985), 391-419.
2. with M. F. Webster, "On the accuracy of finite element and finite difference predictions of non-Newtonian slot pressures for a Maxwell fluid," **J. Non-Newtonian Fluid Mechanics. 25**, pp .93-127 (1987).
3. With M. E. Piesha and M.-R. Liu, "Reversed stability conditions in transient finite element analysis," **Comp. Meths. Appl. Mechs. Eng. 68** pp. 97-114 (1987).
4. With X. Qiu, "Divisor structure of finite element eigenproblems arising from negative and zero masses," **Comp. Meths. Appl. Mechs. Eng. 66**, pp. 365-368 (1988).
5. With R. W. Kolkka, M. G. Hansen, G. R. Lerley, and R. A. Worthing, "Spurt phenomena of the Johnson-Segalman fluid and related models," **J. Non-Newtonian Fluid Mech. 29** pp. 303-335 (1988).
6. With J. Nohel and B. Plohr, "Time-Dependent shear flow of a non-Newtonian fluid," in *Current Problems in Hyperbolic Systems: Riemann Problems and Computations (Bowdoin, 1988)*, **Contemporary Mathematics**, B. Lundquist, editor, Amer. Math. Soc., Providence, RI, to appear, 1989.

### *Other Proceedings Articles Appearing or Accepted During Reporting Period*

7. "A fast algorithm for non-Newtonian flow," in Transactions of the Third Army Conference on Applied Mathematics and Computing, ARO Report #86-1, pp. 651-660, (Atlanta, 1986).

8. A preliminary version of 2. (above), in Proceedings of the Workshop on Computational Fluid Dynamics and Reacting Gas Flows (Minneapolis, 1986), Institute for Math. and Its Applics.
9. A short, preliminary version of 6. (above), in Transactions of the Sixth Army Conference on Applied Mathematics and Computing, to appear (Boulder, 1988).
10. "New transient algorithms for non-Newtonian flows," Proceedings of the 7th Conference on finite Elements in Flow Problems (Huntsville, 1989), to appear.

*Journal Articles Submitted During Reporting Period (in Review)*

11. With J. Nohel and B. Plohr, "Dynamics of shear flow of a non-Newtonian fluid," CMS Technical Summary Report #89-14, 1988 (submitted to **J. Comp. Phys.**).

*Unpublished Reports During Reporting Period*

12. With Minwu Yao, "On hole-pressures in plane Poiseuille flow over transverse slots," MRC Technical Summary Report No. 2943, Mathematics Research Center, University of Wisconsin-Madison (1986).
13. "Computational methods for viscoelastic flow," uncataloged Mathematics Research Center Report, University of Wisconsin-Madison (1987).

*Articles/Reports in Progress*

14. With J. Nohel and B. Plohr, "Phase plane and asymptotic analysis of spurt phenomena," 1989.
15. With Y.-C. Tsai, "Stability analysis of implicit-explicit time integration for viscoelastic flow," 1989.

16. With M. W. Johnson, "On the behavior of the Johnson-Segalman fluid model in step-strains," 1989.

*Thesis by Sponsored Research Assistant*

17. Following are the the title and abstract of the thesis research of Mr. Minwu Yao, whose thesis research has been supported by the current grant. The anticipated completion date of the thesis is Fall, 1989. The abstract is in the form approved by the Thesis Committee at the time of Mr. Yao's preliminary examination (May, 1988):

NUMERICAL SIMULATION  
OF  
PLANAR NEWTONIAN AND NON-NEWTONIAN FLOWS  
BY AN ENHANCED PARTICLE-TRACKING FEM CODE  
by  
MINWU YAO

ABSTRACT

This project concerns computation of numerical solutions for various flow problems of viscoelastic liquids, using an enhanced particle-tracking finite element method (FEM) program - FLUCODE. The capabilities and limitations of this approach are illustrated by in-depth analysis of several flow problems of rheological interest. The code is based on the standard Galerkin FEM formulation and includes numerical techniques that have been developed for many years by D.S. Malkus and his co-workers. The latest version of FLUCODE is now capable of simulating complicated non-Newtonian flows and allows a full range of preprocessing and postprocessing options. The purpose of the work is of two-fold: first is to test and evaluate the numerical techniques used in FLUCODE, to compare our numerical results with the available experimental or other computational data, so as to benchmark the capabilities and limitations of the code and the numerical techniques. The second is to contribute to further understanding of interesting physical problems, such as the

2-D flow over a slot, journal bearing flow and contraction flow. The main topics discussed in this preliminary report include:

- Numerical observation on steady perturbation due to the slot and the excess pressure rise across the slot
- Choice of computational boundary conditions for perturbed Couette flow
- Non-zero driving gradient on the hole centerline and the HPBL prediction
- Spatial decay rate for stationary perturbation of Couette flow
- Introduction to FLUCODE
- Incompressible flows in journal bearings
- Contraction flows.

### *Books*

18. With R. D. Cook and M. E. Plesha, *Concepts and Applications of Finite Element Analysis*, Third Edition, Wiley, 1989.

### **9. Interactions**

#### *Spoken Papers Presented at Meetings, Conferences, Seminars, etc.*

1. Talks at conferences, workshops, and symposia corresponding to items 1., 6., 7., 8., and 9. in the previous section. Item 10. will be presented in April, 1989
2. "Recent progress in computations with single integral models," 4<sup>th</sup> International workshop on Numerical Methods in Non-Newtonian Flows, Spa, Belgium, Jun., 1985.
3. "Zero and negative masses in finite element vibration and transient analysis," Mathematics Department Colloquium, University of Massachusetts-Amherst, Amherst, MA, Oct., 1985.
4. Two-week lecture series on "The finite element method in structural

- and continuum mechanics," Nanjing Aeronautical Institute, Nanjing, P. R. C. (led to Ref. {4}), November, 1985.
5. Same title as 4., Computer Science/Numerical Analysis Seminar, University of Wisconsin, Madison, WI, Dec., 1985.
  6. "Measurement relations for hole pressures and normal stress differences in Rheology," Joint MRC/Applied Math. Seminar, University of Wisconsin, Madison, WI, Feb., 1986.
  7. "Type change in non-Newtonian fluids," Mathematics Department Seminar, Illinois Institute of Technology, Nov., 1986.
  8. Same title as 7., Fluids Research Oriented Group Seminar, Michigan Technological Institute, Houghton, MI, May, 1987.
  9. Numerical aspects of the 'High Weissenberg Number Problem,'" 5<sup>th</sup> International workshop on Numerical Methods in Non-Newtonian Flows, Lake Arrowhead, CA, June, 1987.
  10. "New transient algorithms for non-Newtonian flows," Mathematics Department Seminar, Illinois Institute of Technology, Nov., 1987.
  11. "A stress calculator for BK<sup>2</sup>Z and similar single integral constitutive equations," Annual Meeting of the Society of Rheology, Atlanta, Feb., 1988.

#### *Consultative and Advisory Functions*

1. The P. I. has maintained a close advisory relationship with the non-Newtonian fluids group at Illinois Institute of Technology, headed by B. Bernstein. The pilot method was developed jointly with Bernstein during the six years the P. I. was on the mathematics faculty at I. I. T. The P. I. has been working closely with E. T. Olsen on the development of the stress calculator. The P. I. continues to make regular visits to I. I. T. for the purpose of co-ordinating the research effort. He served on the

Ph. D. Thesis committee of Dr. Alan Altman, who recently received his Ph. D. under E. T. Olsen. His research involved the development of a temperature-dependent material clock for the stress calculator.

2. The P. I. continues to collaborate closely with A. S. Lodge (Dept. Engineering Mechanics, U. W. - Madison), who has developed a laboratory measurement device for normal-stress differences and viscosities based on hole-pressures. The collaboration provides an opportunity for the P. I. to relate his numerical studies to experimental results, and has provided Prof. Lodge with independent verification of the empirical measurement relation upon which his instrument relies.
3. The P. I. continues as a member of the Executive Committee of the Rheology Research Center (U. W. - Madison). This provides a valuable opportunity to interact with a broad spectrum of researchers in non-Newtonian mechanics from Mathematics Chemistry, Engineering Mechanics, and Chemical Engineering.

#### 10. Additional References

1. M. J. Crochet, A. R. Davies, and K. Walters, *Numerical Simulation of Non-Newtonian Flow*, Elsevier, Amsterdam (1984).
2. B. Bernstein, D. S. Malkus, and E. T. Olsen, "A finite element for incompressible plane flows of fluids with memory," *Int. J. Num. Meths. Fluids* 5, pp. 43--70 (1985).
3. B. Bernstein and D. S. Malkus, "Flow of a Curtiss-Bird fluid over a transverse slot using the finite element drift-function method," *J. Non-Newtonian Fluid Mechs* 16, pp. 77-116 (1984).
4. C. F. Curtiss and R. B. Bird, "Kinetic theory for polymer melts. Parts I and II," *J. Chem. Phys.* 74, 2017 (1981).
5. R. B. Bird, O. Hassager, R. C. Armstrong (Vols. I and II), and C. F. Curtiss (Vol. II only), *Dynamics of Polymeric Liquids*, Wiley, New York, (1977).

6. M. W. Johnson and D. Segalman, "A model for viscoelastic fluid behavior which allows non-affine deformation," **J. Non-Newtonian Fluid Mechs.** **2**, 255 (1977).
7. F. Chen and B. Bernstein, "The artificial time drift-function method for finite element techniques for axially symmetric flows of memory fluids," I. I. T. Research Report for NSF Grant MCS 81-02089, 1982.
8. B. Bernstein, "Drift function tracking with compressibility and variable temperature," **J. Non-Newtonian Fluid Mech** **20**, pp 299-321 (1986).
9. A. Altman, Ph. D. Thesis, Department of Mathematics, Illinois Institute of Technology, Chicago, 1987.
10. M. Renardy, "Recent advances in the mathematical theory of steady flow of viscoelastic fluids," **J. Non-Newt. Fluid Mech.** **29**, pp. 11-24 (1988).
11. A. N. Beris, R. C. Armstrong, and R. A. Brown, "Spectral/finite element calculations of the flow of a Maxwell fluid between eccentric rotating cylinders," **J. Non-Newtonian Fluid Mech.** **22**, pp. 129-167 (1988).
12. R. C. King, M. R. Apelian, R. C. Armstrong, and R. A. Brown, "Numerically stable finite element techniques for viscoelastic calculations in smooth and singular geometries," **J. Non-Newtonian Fluid Mech.**, to appear, 1988.
13. S. Burdette, Ph. D. Thesis, Department of Chemical Engineering, University of Wisconsin, Madison, 1987.
14. A. S. Lodge and L. de Vargas, "Positive hole pressures and negative exit pressures generated by molten low-density polyethylene flowing through a slit die," **Rheologica Acta** **22**, p. 51 (1983).
15. K. Higashitani and W. G. Pritchard, "A kinematic calculation of intrinsic errors in measurements made with holes," **Trans. Soc. Rheol.** **16**, pp. 687-696 (1972).

16. R. Srinivasan, "The hole-pressure problem: on the Higashitani-Pritchard theory for transverse and axial slots," **Rheologica Acta**, **26**, pp. 107-118 (1987).
17. T. Cochrane, K. Walters, and M. F. Webster, "On Newtonian and non-Newtonian flow in complex geometries," **Phil. Trans. Roy. Soc. London** **301**, pp. 163-181 (1981).
18. T. J. R. Hughes, W. K. Liu, and A. Brooks, "Finite element analysis of incompressible viscous flows by the penalty function formulation," **J. Comp. Phys.** **30**, pp. 1--60 (1979).
19. J. K. Hunter and M. Slemrod, "Viscoelastic fluid flow exhibiting hysteretic phase changes," **Phys. Fluids** **26**, pp. 2345--2351 (1983).
20. M. M. Denn, *Process Fluid Mechanics*, Prentice-Hall, Englewood Cliffs, 1980.
21. F. Sugeng, N. Phan-Thien, and R. I. Tanner, A boundary element investigation of the pressure-hole effect, **J. Rheol.** **32**, pp. 215-233 (1987).
22. M. S. Engelman, "FIDAP -- A fluid dynamics analysis package," **Adv. Software Engng.** **4**, p. 163 (1982).

RESUMÉ

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Professor of Engineering Mechanics and Affiliate Member, Center for the Mathematical Sciences (formerly Mathematics Research Center), University of Wisconsin - Madison.

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Associate Professor of Mathematics, Illinois Institute of Technology, August, 1982 --- December, 1983.

Assistant Professor of Mathematics, Illinois Institute of Technology, August, 1977 --- August, 1982.

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**Research Areas:**

Finite element analysis of non-Newtonian flow. Theory and error analysis of the finite element method with constraints --- incompressible fluid/solid mechanics problems, and structural problems with shear constraints. Development of finite element procedures for nonlinear elasticity. Finite element methods for elastodynamics and structural dynamics.

### **Professional Society Memberships:**

Mathematical Methods Committee of the American Society of Civil Engineers --- Engineering Mechanics Division (non-ASCE member affiliate), Society for Industrial and Applied Mathematics, Society of Rheology

### **Education:**

Ph. D.: Boston University, Boston, MA (1976).  
M. A.: Boston University, Boston, MA (1975).  
B. A.: Yale University, New Haven, CT (1968).  
Secondary: Middlesex School, Concord, MA (1963)

### **Personal:**

Date of Birth: June 30, 1945.  
Marital Status: Married (to Evelyn Rockar Malkus, December, 1977).  
Children: Four --- Christopher (b. Sept., 1980), Annelise (b. Dec., 1982), Byron (b. Mar., 1985), Renata (b. Mar., 1985).

### **Publications:**

1. With I. Fried, "Finite element mass matrix lumping by numerical integration with no convergence rate loss" (**Int. J. Solids and Struct.**, **11**, pp. 461-466, 1975).
2. "A finite element displacement model valid for any value of the compressibility" (**Int. J. Solids and Struct.** **12**, pp. 731-738, 1976).
3. With T. J. R. Hughes, "Mixed finite elements --- reduced and selective integration techniques: A unification of concepts" (**Comp. Meths. Appl. Mechs. Eng.** **15**, pp. 63-81, 1978).
4. "Penalty methods in finite element analysis of fluids and structures" (**Nuc. Engng. Design** **57**, pp. 441-448, 1980).
5. "Finite elements with penalties for nonlinear elasticity" (**Int. J. Num. Meths. Engng.** **16**, pp. 121-136, 1980).
6. With E. R. Fuller, Jr., "An isoparametric finite element model for large-strain elastostatics" (**J. Res. N. B. S.** **86(1)**, pp. 79-109, 1981).
7. With B. Bernstein and M. K. Kadiyar, "Steady flow of memory fluids with finite elements: two test problems" (**Comp. Meths. Appl. Mechs. Eng.** **27**, pp. 279-302, 1981).

8. "Functional derivatives and finite elements for the steady spinning of a viscoelastic filament" (**J. Non-Newtonian Fluid Mechs.** **8**, pp. 223-237, 1981).
9. "Eigenproblems associated with the discrete LBB condition for incompressible finite elements" (**Int. J. Engng. Sci.** **19**, pp. 1299-1310, 1981).
10. With R. T. Haftka, "Calculation of sensitivity derivatives in thermal problems by finite differences" (**Int. J. Num. Meths. Engng.** **17**, pp. 1811-1821, 1981).
11. With T. J. R. Hughes, "A general penalty/mixed equivalence theorem for anisotropic, incompressible finite elements" (in **Hybrid and Mixed Finite Element Methods**, S. N. Atluri, R. H. Gallagher, and O. C. Zienkiewicz, eds., Wiley, New York, 1983, pp. 487-496).
12. With E. T. Olsen, "Obtaining error estimates for optimally constrained incompressible finite elements" (**Comp. Meths. Appl. Mechs. Eng.** **42**, pp. 331-353, 1984).
13. With B. Bernstein, "Flow of a Curtiss-Bird fluid over a transverse slot using the finite element drift-function method" (**J. Non-Newtonian Fluid Mechs.** **16**, pp.77-116, 1984).
14. With B. Bernstein and E. T. Olsen, "A finite element for incompressible, plane flows of fluids with memory" (**Int. J. Num. Meths. Fluids** **5**, pp. 43-70, 1985).
15. "Finite element simulation of flows of fluids with integral constitutive equations" (**Comm. Appl. Num. Meth.** **1**, pp. 275-280, 1985).
16. "Finite element methods for viscoelastic flow" (**Viscoelasticity and Rheology**, A. S. Lodge, M. Renardy, and J. A. Nohel, eds., Academic Press, Orlando, pp. 391-419).
17. With M. E. Plesha, "Zero and negative masses in finite element vibration and transient analysis" (**Comp. Meths. Appl. Mechs. Eng.** **59**, pp. 281-306, 1986).
18. With M. F. Webster, "On the accuracy of finite element and finite difference predictions of non-Newtonian slot pressures," (**J. Non-Newtonian Fluid Mechs.** **25**, pp. 93-127, 1987).
19. With M. E. Plesha and M.-R. Liu, "Reversed Stability conditions in finite element transient analysis," (**Comp. Meths. Appl. Mechs. Eng.** **68**, pp. 97-114, 1988).
20. With X. Qiu, "Divisor structure of finite element eigenproblems

arising from negative and zero masses," **Comp. Meths. Appl. Mechs. Eng.** **66**, pp. 365-368, 1988.)

21. With R. W. Kolkka, M. G. Hansen, G. R. Ierley, and R. A. Worthing, "Spurt phenomena of the Johnson Model fluid and related models" (**J. Non-Newtonian Fluid Mechs.** **25**, pp. 93-127, 1988).

#### **Books:**

1. Chapter length Appendix II to Chap. IV of a new textbook by T. J. R. Hughes: **The Finite Element Method: Linear Static and Dynamic Analysis**, Prentice-Hall, 1987.
2. With R. D. Cook and M. E. Plesha: **Concepts and Applications of Finite Element Analysis**, Third Edition, Wiley, 1989.

#### **Other Publications:**

1. With John A. Nohel, and Bradley J. Plohr, "Time-dependent shear flow of a non-Newtonian fluid," in *Current progress in Hyperbolic Systems: Riemann Problems and Computations (Bowdoin, 1988)*, **Contemporary Math.**, B. Lundquist, ed., Amer. Math. Soc., Providence, R.I., to appear, 1989.
2. "New transient algorithms for non-Newtonian flows," *7th Conf. on Finite Element Methods in Flow Problems (Huntsville, 1989)*, T. J. Chung, ed., to appear.

#### **Publications in Progress**

1. With John A. Nohel and Bradley J. Plohr, "Phase Plane and Asymptotic Analysis of Spurt Phenomena."
2. With Millard W. Johnson, "On the Behavior of the Johnson-Segalman Model in Step-Strains."
3. With Y.-C. Tsai, "Stability Analysis of Implicit-Explicit Time Integration for Viscoelastic Flow."

#### **Recent Technical Reports**

1. "A fast algorithm for non-Newtonian flow" (MRC Technical Summary Report No. 2860, Mathematics Research Center, University of Wisconsin, 1985).
2. "Calibration of hole-pressure measurements in non-Newtonian flow by numerical methods" (MRC Technical Summary Report No. 2863, Mathematics Research Center, University of Wisconsin, 1985).
3. With Minwu Yao, "On hole pressures in plane Poiseuille flow over

transverse slots" (MRC Technical Summary Report No. 2943, Mathematics Research Center, University of Wisconsin, 1986).

4. With John A. Nohel and Bradley J. Plohr, "Dynamics of shear flow of a non-Newtonian fluid" (CMS Technical Summary Report No. 89-14, Center for the Mathematical Sciences, University of Wisconsin, 1988), Also submitted to *J. Comp. Phys.*

## Current and Pending Support for David S. Malkus

### I. CURRENT

1) New Transient and Pseudo-Transient Algorithms for Viscoelastic Materials

Agency: AFOSR

Amount: \$111,330

Duration: 24 months

Starting Date: 12/15/88

Man Months: P. I. 1 month (Summer), 2 R. A.s 2 years

Location of Work: University of Wisconsin - Madison

2) Interdisciplinary Research in Viscoelasticity and Rheology (with J. Nohel)

Agency: ARO

Amount: \$180,000

Duration: 3 Years

Starting Date: 5/23/87

Man Months: 14% acad. year support for Malkus

Location of Work: University of Wisconsin - Madison

3) Interdisciplinary Research in Viscoelasticity and Rheology (with J. Nohel)

Agency: AFOSR

Amount: \$40,500

Duration: 1 Year

Starting Date: 6/1/88

Man Months: 1 half-time R. A., 1 half time Post-Doc.

Location of Work: University of Wisconsin - Madison

4) Modelling, Analysis and Computation in Viscoelasticity (with J. Nohel and B. Plohr)

Agency: NSF

Amount: \$182,764

Duration: 2 Years

Starting Date: 8/1/87

Man Months: 8% acad. year support (both years) and 2 mos.

Summer (2nd year) for Malkus

Location of Work: University of Wisconsin - Madison

II. PENDING

1) Interdisciplinary Research in Viscoelasticity and Rheology (with J. Nohel)

Agency: AFOSR

Amount: \$40,500

Duration: 1 Year

Starting Date: 6/1/89

Man Months: 1 half-time R. A., 1 half time Post-Doc.

Location of Work: University of Wisconsin - Madison

2) Modelling, Analysis and Computation in Viscoelasticity (with J. Nohel and B. Plohr)

Agency: NSF

Amount: \$642,936

Duration: 3 Years

Starting Date: 9/1/89

Man Months: 8% acad. year support (3 years) 1 mo.

Summer (first year) and 2 mos. Summer (2nd and third

year) for Malkus. 2 half-time R. A.s, 1 Post-Doc. (3 years).

Location of Work: University of Wisconsin - Madison