IWNMNNF 2007

XV^th International Workshop on Numerical Methods for Non-Newtonian Flows

June 6-10, 2007, Rhodes, Greece

Book of Abstracts

FORTH/ICE-HT **University of Patras** **Hellenic Society of Rheology**

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CHAIRS' MESSAGE

It is with great pleasure that we welcome all delegates and accompanying persons to the XVth International Workshop on Numerical Methods for Non-Newtonian Flows (XVth IWNMNNF-2007) on the island of Rhodes, Greece. Since their inception in 1979, in Providence, Rhode Island, USA, the workshops are rotated biennially between North America and Europe. This is the first time the meeting is being held in Greece. Rhodes island is a proper destination as the meetings have come a full circle after almost 30 years of frantic activity, which have seen workshop meetings in castles, lakes, islands, seasides, etc. Rhodes, as the capital of the Dodecanese Islands, combines all of the above, and has been a place of tourism and holidays since antiquity.

The XVth IWNMNNF is by all measures a truly international event, drawing scientists and engineers from 20 countries around the world. The Workshop includes a plenary lecture and 7 thematic sessions. A total number of 60 papers have been divided into two categories: 50 oral and 10 posters. We hope that this Workshop will promote and facilitate scientific exchange, collaboration and interactions between participants as well as their organisations in advancing non-Newtonian Fluid Mechanics and Computational Rheology to higher levels of success.

Rhodes is reputed as the "Island of the Sun" and boasts some terrific beaches together with ancient and medieval sights that attract people from around the world. We hope all international delegates will experience the important attractions that Rhodes has to offer during their stay on the island.

We thank all the sponsors of this Workshop for their generous support. We are indebted to the members of the Organising and Scientific Committees and other individuals (Ms. K. Zacharopoulou, Ms. M. Calliamvakou, and Ms. S. Sofou) for their commitment and hard work in order to make this Workshop a successful event.

Prof. Evan Mitsoulis
Workshop Chair

Prof. Vlasis Mavrantzas
Workshop Vice-Chair

IWNMNNF 2007 Program

Day 1: Wednesday Afternoon, June 6, 2007

18:00-18:30 *Registration*
18:30-18:40 Welcome remarks – Motivation – Organizational details
Evan Mitsoulis, National Technical University of Athens, Greece

Plenary Lecture

Chair: E. Mitsoulis

18:40-19:20 The changing face of computational rheology
Roger Tanner, University of Sydney, Sydney, NSW, Australia

Session 1: Viscoelastic Suspensions

Chair: B. Khomami

19:25-19:45 (A24) Rigid rods in non-homogeneous shear flow
M.J. Green, R.C. Armstrong, MIT, Cambridge, MA, USA
R.A. Brown, Boston University, Boston, MA, USA

19:50-20:10 (A30) Numerical simulations of concentrated viscoelastic suspensions in an elongational flow
G. D′Avino, P.L. Maffetone, University of Napoli, Italy
M.A. Hulsen, G.W.M. Peters, Eindhoven University of Technology, The Netherlands

20:15-20:35 (A23) Numerical simulation of polymer melts containing short and long fibers
P. Wapperom, D.G. Baird, G. Velez, A.P.R. Eberle, Virginia Tech, Blacksburg, VA, USA

20:40-21:00 (A70) Numerical simulation of suspensions of rigid and deformable particles in polymer melts
Ahamadi Malidi, O.G. Harlen, University of Leeds, UK

21:05-22:30 *Welcome buffet – Registration (cont.)*

Day 2: Thursday Morning, June 7, 2007

Session 2: Multiscale Modeling and Molecular Simulations
Chair: V.G. Mavrantzas

8:00-8:20	(A45) Realizing rheological dreams: efficient solution of highly dimensional Fokker-Planck equations A. Ammar, Laboratoire de Rheologie, Grenoble, France F. Chinesta, ENSAM, Paris, France R. Keunings, Université Catholique de Louvain, Louvain-la-Neuve, Belgium
8:25-8:45	(A20) Optimal choices of correlation operators in Brownian simulation methods Raz Kupferman, Yossi Shamai, The Hebrew University, Jerusalem, Israel
8:50-9:10	(A9) A log transformation applied to the method of Brownian configuration fields Claude Mangoubi, Raz Kupferman, The Hebrew University, Jerusalem, Israel Martien A. Hulsen, Eindhoven University of Technology, The Netherlands
9:15-9:35	(A11) A P3M method for computation of many-body hydrodynamic interactions in a confined geometry: application to migration and apparent slip in nondilute polymer solutions J.P. Hernandez-Ortiz, S. Anekal, M.D. Graham, University of Wisconsin-Madison, USA
9:40-10:00	(A78) Frictional drag properties of polymeric solution in complex kinematics flows: a multi-scale simulation approach A.P. Koppol, R. Sureshkumar, Washington University, St. Louis, MO, USA B. Khomami, University of Tennessee, Knoxville, TN, USA
10:05-10:20	*Coffee break*

Session 3: Multiscale Modeling and Molecular Simulations (Cont'd)
Chair: R. Keunings

10:20-10:40	(A34) DPD as a tool for rheological characterization T.F. Clarke, R.C. Armstrong, MIT, Cambridge, MA, USA
10:45-11:05	(A73) Atomistic Monte-Carlo simulation of a polymer melt under a flow field by employing generalized ensembles Chunggi Baig, V.G. Mavrantzas, University of Patras, Greece; FORTH-ICE/HT, Patras, Greece

11:10-11:30 (A6) Rheological and Entanglement Characteristics of Linear Chain Polyethylene Liquids in Planar Couette and Planar Elongational Flows
J.M. Kim, D.J. Keffer, B.J. Edwards, University of Tennessee, USA
M. Kröger, ETH, Zurich, Switzerland

11:35-12:00 (A42) Transient 3D Flow of Polymer Solutions
N.F. Morrison, J.M. Rallison, University of Cambridge, UK

12:05-14:00 *Lunch*

Day 2: Thursday Afternoon, June 7, 2007

Session 4: Viscoplastic Fluids – Modeling and Simulations

Chair: A.N. Beris

14:00-14:20 (A49) Steady bubble rise and deformation in Bingham fluids and conditions for their entrapment
J. Tsamopoulos, Y. Dimakopoulos, N. Chatzidai, G. Karapetsas, M. Pavlidis, University of Patras, Greece

14:25-14:45 (A76) Weakly compressible Poiseuille flows of a Bingham fluid
E. Taliadorou, G. Georgiou, A. Alexandrou, University of Cyprus, Nicosia, Cyprus

14:50-15:10 (A79) Numerical simulation of calendering of viscoplastic materials
E. Mitsoulis, S. Sofou, National Technical University of Athens, Greece

15:15-15:35 (A59) Wave evolution in two-layer pressure driven flow – Newtonian upper layer over a non-Newtonian bottom layer
P. Valluri, P.D.M. Spelt, O.K. Matar, C.J. Lawrence, Imperial College London, UK

15:40-15:55 *Coffee break*

15:55-16:15 (A85) Squeeze flow of carbopol gels
E. Mitsoulis, I. Argyropaidas, National Technical University of Athens, Greece

16:20-16:40 (A63) Blood hemodynamics in carotid bifurcation: influence of rheological models
P. Ternik, Z. Zunic, J. Marn, University of Maribor, Slovenia

16:45-17:00 Discussion

Free Evening

Day 3: Friday Morning, June 8, 2007

Session 5: Viscoelastic Flow Instabilities

Chair: P.J. Oliveira

8:00-8:20 (A8) Using Newton-GMRES for viscoelastic flow time-steppers
Z. Anwar, R.C. Armstrong, MIT, Cambridge, MA, USA

8:25-8:45 (A46) On a new elastic instability: bifurcation in a cross-slot
R.J. Poole, University of Liverpool, UK
M.A. Alves, University of Porto, Portugal
P.J. Oliveira, University of Beira Interior, Covilha, Portugal

8:50-9:10 (A72) Bifurcation analysis of flow instabilities in polymer melts during extrusion
M.E. Kavousanakis, C.I. Siettos, A.G. Boudouvis, National Technical University of Athens, Greece
L. Russo, University of Naples, Italy
G. Georgiou, University of Cyprus, Nicosia, Cyprus

9:15-9:35 (A31) Modeling of axisymmetric instabilities observed during the electrospinning of highly conducting, non-Newtonian jets
C.P. Carroll, Y.L. Joo, Cornell University, Ithaca, NY, USA

9:40-10:00 (A53) Cavity filling process modeling by rheological characterization and large scale computation
K. Christodoulou, R. Mehrabi, A. Mehrabi, E. Rozenbaum, Avery Research Center, Pasadena, CA, USA

10:05-10:20 *Coffee break*

Session 6: Viscoelastic Flow Instabilities (Cont'd)

Chair: G.C. Georgiou

10:20-10:40 (A52) A parallel adaptive unstructured finite volume method for linear stability (normal mode) analysis of viscoelastic fluid flows
M. Sahin, H.J. Wilson, University College London, UK

10:45-11:05 (A9) A new stability mechanism associated with the Oldroyd-B model in creeping flow regime
Raz Kupferman, The Hebrew University, Jerusalem, Israel

11:10-11:30 (A54) Coil-stretch transition and the break down of continuum models
M. Bajaj, J. Ravi Prakash, Monash University, Melbourne, Australia
M. Pasquali, Rice University, Houston, TX, USA

11:35-11:55 (A15) On kinetic models for dilute suspensions of rigid rods
F. Otto, University of Bonn, Germany

A. Tzavaras, University of Maryland, MD, USA

12:00-14:00 *Lunch*

Day 3: Friday Afternoon, June 8, 2007

Session 7: Poster Session

14:00-15:40 **P1**. (A74) A generalized single-conformation tensor viscoelastic model based on principles of non-equilibrium thermodynamics
P. Stephanou, Chunggi Baig, V.G. Mavrantzas, University of Patras, Greece

P2. (A58) Numerical simulation of complex fluid flows with non-Newtonian differential models
O. Wuensch, M. Krebs, University of Kassel, Germany

P3. (A57) Numerical simulations of flow in a variable speed co-rotating twin screw extruder
C. Tzoganakis, S. Zhu, University of Waterloo, Canada
T. Shigeishi, K. Tikara, Japan Steel Works, Hiroshima, Japan

P4. (A48) Correlating the rheology of PVC pastes with particle characteristics
M.G. Rasteiro, L.M. Ferreira, A. Tomàs, S. Figueiredo, University of Coimbra, Portugal

P5. (A80) Rheological characterization of foodstuff used in rolling experiments and modeling via integral constitutive equations
E. Muliawan, S.G. Hatzikiriakos, University of British Columbia, Vancouver, Canada
S. Sofou, E. Mitsoulis, National Technical University of Athens, Greece

P6. (A81) Predicting the behaviour of nylon-6 through industrial spin packs
A. Gustin, A. Zupancic, University of Ljubljana, Slovenia
E. Mitsoulis, National Technical University of Athens, Greece

P7. (A71) Numerical simulation of the extrusion of strongly compressible liquid foams
E. Taliadorou, G. Georgiou, University of Cyprus, Nicosia, Cyprus
E. Mitsoulis, National Technical University of Athens, Greece

P8. (A77) Annular Poiseuille flow of a Newtonian liquid with non-monotonic slip along the walls
M. Chatzimina, G. Georgiou, University of Cyprus, Nicosia, Cyprus
K. Housiadas, University of the Aegean, Samos, Greece
S.G. Hatzikiriakos, University of British Columbia, Vancouver, Canada

P9. (A41a) Comparative study of multi-mode constitutive equations for film blowing process
S. Sarafrazi, F. Sharif, Amirkabir University of Technology, Tehran, Iran

P10. (A82) The temperature dependence of the Rouse mode relaxation spectrum and zero shear rate viscosity in cis-1,4-polybutadiene: results from long atomistic molecular dynamics simulations down to the glass transition temperature T_g
G. Tsolou, V.G. Mavrantzas, University of Patras, Greece

15:40-15:55 *Coffee break*

16:00-20:30 *Excursion to Ancient Lindos*

Day 4: Saturday Morning, June 9, 2007

Session 8: Viscoelastic Fluids - Modeling and Simulations

Chair: J. Tsamopoulos

8:00-8:20 (A47) On the gas penetration in periodically constricted circular tubes filled with viscoelastic liquids
Y. Dimakopoulos, J. Tsamopoulos, University of Patras, Greece

8:25-8:45 (A27) The log-conformation tensor approach in the FVM framework: benchmark solutions and stability analysis
A. Afonso, M.A. Alves, University of Porto, Portugal
F.T. Pinho, University of Minho, Braga, Portugal
P.J. Oliveira, University of Beira Interior, Covilha, Portugal

8:50-9:10 (A13) Oscillating channel flows of UCM and Oldroyd-B fluids: numerical and analytical solutions
A.S.R. Duarte, A.I.P. Miranda, P.J. Oliveira, University of Beira Interior, Covilha, Portugal

9:15-9:35 (A39) Numerical simulation of the flow of a PTT fluid past a cylinder
H. Kamal, L. Thais, G. Mompean, H. Naji, Polytech′Lille, France

9:40-10:00 (A84) On the numerical treatment of integral models for elasticity in a compressible fluid
P.C Bollada, T.N. Phillips, Cardiff University, UK

10:05-10:20 *Coffee break*

Session 9: Viscoelastic Fluids - Modeling and Simulations (cont'd)

Chair: E. Mitsoulis

10:20-10:40 (A51) Viscoelastic analysis of complex flows: from the constitutive model through the numerical simulations and their experimental validation
I. Sirakov, University of St-Etienne, France
E. Mitsoulis, National Technical University of Athens, Greece

10:45-11:05 (A50) Numerical simulation of viscoelastic flows in cross-slot flow devices
M.F. Webster, F. Belblidia, B. Puangkird, University of Wales, Swansea, UK

11:10-11:30 (A19) Prediction of die swell in polymer melt extrusion using an Arbitrary Lagrangian Eulerian (ALE) based finite element method
V. Ganvir, A. Lele, Pune, India
R. Thaokar, IIT, Bombay, India
B.P. Gautham, NCL, Pune, India

11:35-11:55 (A41b) Non-isothermal simulation of the film-blowing process using the multi-mode extended pom-pom model
S. Sarafrazi, F. Sharif, Amirkabir University of Technology, Tehran, Iran

12:00-14:00 *Lunch*

Day 4: Saturday Afternoon, June 9, 2007

Session 9: Complex Materials: Experiments and Modeling
Chair: M.F. Webster

14:00-14:20 (A22a) Computing with power-law viscoelastic materials
Roger Tanner, F. Qi, S.-C. Dai, University of Sydney, NSW, Australia

14:25-14:45 (A68) Characterization of the compressive behaviour of brain tissue and constitutive modeling
G.W.M. Peters, M. Hrapko, J.A.W. van Dommelen, J.S.H.M. Wismans, Eindhoven University of Technology, The Netherlands

14:50-15:10 (A43) Experimental and numerical evaluation of drop deformation and break-up in complex flow fields
R.D. Egholm, P. Szabo, Technical University of Denmark, Lyngby, Denmark
P. Fischer, ETH, Zurich, Switzerland
K. Feigl, Michigan Technological University, Houghton, MI, USA

15:15-15:35 (A67) Experimental and numerical study of cavitation in journal bearings
P.C. Bollada, T.N. Phillips, Cardiff University, UK
P.R. Williams, R.L. Williams, University of Wales, Swansea, UK

15:40-15:55 *Coffee break*

Session 10: Complex Materials: Experiments and Modeling (Cont'd)
Chair: G.W.M. Peters

15:55-16:15 (A26) Modeling of non-isothermal electrospinning of polymer melts with and without crystallization
E. Zhmayev, Y.L. Joo, Cornell University, Ithaca, NY, USA

16:20-16:40 (A37) Structure-property relationships for the Newtonian and the non-Newtonian flow of polymer solutions
F. Meyer, H. Storz, J. Storz, A. Bingoel, W.-M. Kulicke, University of Hamburg, Germany

16:45-20:30 *Free time*

20:30-22:30 *Conference dinner*

Day 5: Sunday Morning, June 10, 2007

Session 11: Turbulence in Complex Fluids
Chair: G. Mompean

9:00-9:20 (A56) Dynamic K-L analysis of coherent structures based on DNS of turbulent Newtonian and viscoelastic flows
G. Samanta, A.N. Beris, University of Delaware, Newark, DE, USA
G. Oxberry, MIT, MA, USA
R. Handler, Naval Research Laboratory, Washington, DC, USA
K. Housiadas, University of the Aegean, Samos, Greece

9:25-9:45 (A55) A log-exponential mapping for the preservation of positive definiteness in the numerical integration of viscoelastic constitutive equations
K. Housiadas, University of the Aegean, Samos, Greece
L. Wang, A.N. Beris, University of Delaware, Newark, DE, USA

9:50-10:10 (A38) Direct and large eddy numerical simulations of FENE-P drag reduction flows
L. Thais, G. Mompean, Polytech′Lille, France
A.E. Tejada-Martinez, University of South Florida, FL, USA
T.B. Gatski, University of Poitiers, ENSMA, France

10:15-10:35 (A29) A turbulence closure for viscoelastic fluids based on the FENE-P model
F.T. Pinho, University of Minho, Braga, Portugal
P.R. Resende, University of Porto, Portugal
C.F. Li, R. Sureshkumar, Washington University, St. Louis, MO, USA
B.A. Younis, University of California, Davis, CA, USA

10:35-11:00 *Coffee break*

11:00-11:20 (A21) DNS experiments of surfactant drag reducing fluid flows
S. Guillou, R. Makhloufi, F. Hadri, A. Besq, University of Cherbourg, France

11:25-11:55 Discussion – Closing remarks

12:00-14:00 *Lunch*

END OF WORKSHOP

PLENARY LECTURE

The Changing Face of Computational Rheology

Roger Tanner

Department of Aeronautics, University of Sydney, Australia

The Workshop has now been in operation since the first meeting in Providence, Rhode Island, in 1979. We are now in a full circle on Rhodos Island, and this talk will survey progress and changes that have occurred in nearly forty years of furious activity .The development of computer power has followed Moore's Law, and we can now begin to decide whether or not computational rheology has kept pace with this. New aspects of our subject continue to appear, and speculation about the future will close the presentation.

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ORAL CONTRIBUTIONS

Rigid Rods in Nonhomogeneous Shear Flow

M.J. Green [1], R.C. Armstrong [2], R.A. Brown [3]

[1] Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA
[2] Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA
[3] Boston University, Boston, MA, USA

A generalized numerical framework is developed for the simulation of rodlike particles in nonhomogeneous shear flow. Although the time-periodic behavior of rigid rods is well-characterized for homogeneous shear flow, rod dynamics in nonhomogeneous shear flow are poorly understood. Continuum elastic theories of structure evolution lack the ability to describe domain formation and interfacial motion, while the simplified Doi molecular theory predicts an aphysical texture buildup in pressure-driven nonhomogeneous shear flow. Our method avoids these simplifications through a finite-element discretization of the full nonhomogeneous Doi diffusion equation for the rod distribution function with no closure approximations. The dynamic simulation uses a discretized form of the full nonhomogeneous Onsager intermolecular potential, which accurately captures excluded-volume interactions of the rods in order to resolve thin interfaces between domains. This parallel, semi-implicit time-stepper also utilizes an operator-splitting technique to decouple the calculation of the liquid-crystalline contribution to the stress from the velocity field update.

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Numerical simulations of concentrated viscoelastic suspensions in an elongational flow

G. D'Avino [1], P.L. Maffettone [1], M.A. Hulsen [2], G.W.M. Peters [2]

[1] Dipartimento di Ingegneria Chimica, Università Federico II di Napoli, Piazzale, Tecchio 80, I-80125, Napoli, ITALY
[2] Department of Mechanical Engineering, Eindhoven University of Technology, Eindhoven 5600 MB, The Netherlands

Stretching of polymer melts is quite common in several industrial processes like thermoforming, fiber spinning and blow molding. Thus, the elongational viscosity of polymers plays a crucial role in predicting the properties of the final products. The presence of an inclusion locally modifies the imposed elongation flow and partially suppresses strain hardening. In order to predict the observed features we have developed a two-dimensional numerical model of planar elongational flow accounting for viscoelasticity of the suspending fluid.
The numerical scheme is based on the DEVSS-G/SUPG technique combined with the recently developed log-conformation representation (LCR) to improve numerical stability of the computation of the conformation tensor at high Weissenberg numbers. The particles are treated as rigid disks and are implemented with a rigid ring constraint in a fictitious domain approach. A three-layer domain is considered in order to use a fixed and time-independent mesh. The microscopic structure of the suspension has been investigated and the impact of the presence of inclusions on the local fields is analyzed. In particular, for high Weissenberg numbers, highly oriented stretched regions are observed. Furthermore, our simulations show an increasing bulk elongational viscosity with the Weissenberg number as well as with particle area fraction. However, the strain hardening decreases if the particle area fraction increases, in qualitative agreement with the behavior seen in experiments.

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Numerical Simulation of Polymer Melts Containing Short and Long Fibers

P.Wapperom [1], D.G. Baird [2], G. Velez [3], A.P.R. Eberle [2]

[1] Dept. of Mathematics, Virginia Tech, Blacksburg, VA, USA
[2] Dept. of Chemical Engineering, Virginia Tech, Blacksburg, VA, USA
[3] Dept. of Macromolecular Science and Engineering, Virginia Tech, Blacksburg, VA, USA

In order to use thermoplastics to manufacture parts, it is necessary to reinforce them with short or long fibers. The mechanical properties of the thermoplastic composite is highly dependent on the orientation of the fibers.
In this talk we study by way of numerical simulation the orientation of short and long glass fibers in a polymeric matrix. The fibers are modeled using Doi theory for rigid rod molecules, while a Phan-Thien/Tanner constitutive equation is used for the polymer matrix. Material parameters are obtained by fitting the model to dynamic and steady shear measurements. The Doi/PTT model will be evaluated in rheometrical flow (intermittent stress growth experiments) and complex flows (flow through a center-gated disk).
The numerical technique consists of a standard finite element approximation for the equations of motion and mesh and a discontinuous Galerkin finite element method for the constitutive equations. Predictions of the fiber orientations will be compared with experimental results.

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Numerical Simulations of Suspensions of Rigid and Deformable Particles in Polymer Melts

Ahamadi Malidi, O.G. Harlen

University of Leeds, UK

In many polymer processing applications filler particles are added to the polymer matrix. To study the rheology of such multiphase systems we perform direct simulations of the motion of the suspended particles when subjected to an external flow, such as simple shear or planar extensional flow. For convenience of numerical simulation, the infinite domain is approximated by a spatially periodic structure based upon a unit cell containing a limited number of particles. The numerical methodology adopted to solve the viscoelastic flow is based on the Lagrangian-Eulerian method of Harlen et al. A quotient map representation, in which each point in the unit cell is replicated at corresponding image points in the lattice, is used to impose the spatially periodic structure. For shear flow this is equivalent to the Lees-Edwards boundary condition, and in planar extensional flow we use the Kraynik-Reinelt self replicating lattice. For rigid particles the boundary conditions are imposed via a surface density force, which acts as a Lagrange multiplier to force the fluid inside the particles to behave as a rigid solid. For elastic particles we compute the deformation inside the particle using different constitutive models inside and outside the particle. In shear flow our simulations results are in quantitative agreement with rheological measurements on suspensions of glass spheres in polystyrene melts.

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Realizing Rheological Dreams: Efficient Solution of Highly Dimensional Fokker-Planck Equations

A. Ammar [1], F. Chinesta [2], R. Keunings [3]

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[2] LMSP, ENSAM Paris, France
[3] CESAME, Université Catholique de Louvain, Belgium

Kinetic theory models involving the Fokker-Planck equation can be accurately solved using a mesh support. However, that involves a high number of approximation functions. In the finite element framework, widely used in complex flow simulations, each approximation function is related to a node that defines the associated degree of freedom in the configuration space.
For highly configuration space dimensions, standard discretization fails to describe the solution using a deterministic approach because of the high number of degrees of freedom involved in the simulation (that could reach astronomical values, e.g. 10^{300} or more˜ remember that 10^{80} corresponds to the presumed number of elementary particles in the universe).
The strategy proposed in this work allows circumventing this drawback by using a reduced approximation basis within an adaptive procedure making use of an efficient separation of variables. The idea is to dissociate the configuration space in some elementary spaces and to build some appropriate functions over these reduced spaces. The weak formulation related to the kinetic theory description (Fokker-Planck equation) is then discretized allowing writing the solution as a sum of different space functions products. In this approach, time and physical space can be associated to the configuration space as additional dimensions avoiding incremental procedures. This method has been applied in our former works to describe Multi-Bead-Spring models, polymer melt, fiber suspensions, heat transfer in heterogeneous media, etc, but it could be applied to any model concerned by the curse of dimensionality. The main ideas and results will be revisited in this work that also focuses in some new potentialities.

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Optimal Choices of Correlation Operators in Brownian Simulation Methods

Raz Kupferman [1], Yossi Shamai [1]

[1] Institute of Mathematics, The Hebrew University, Jerusalem, Israel

Brownian simulation methods have become very popular in the context of polymeric fluids since the 1990s, with the introduction of simulation methods such as CONFFESSIT and Brownian configuration fields (BCF). To some extent, these two methods can be viewed as instances of the same technique, differing only in the choice of the spatial correlation function of the noise. Pioneering work of Lelievre, Lebris and co-workers derives, in specific example, an optimal noise correlation that minimizes the variance of the resulting computations. In this lecture, we will present a general formulation of variance minimization and optimal noise correlation. We will show that the resulting optimization problem is of a type amenable to an algorithmic solution. Specific examples will be considered and general considerations will be exposed.

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A log Transformation Applied to the Method of Brownian Configuration Fields

Claude Mangoubi [1], Raz Kupferman [1], Martien A. Hulsen [2]

[1] Institute of Mathematics, The Hebrew University, Jerusalem, Israel
[2] Department of Mechanical Engineering, Eindhoven University of Technology, The Netherlands

The log-C transformation applied to differential constitutive equations has drastically improved their numerical stability [1,2]. It has allowed computations at significantly higher Weissenberg numbers than previously. The accuracy of the solutions and convergence upon mesh refinement at high Wiesenberg number is still an open question, however.
The method of Brownian configuration fields (BCF) [3] is currently the preferred method for simulating fluid flow with FENE-type stochastic models. BCF is known to be more numerically stable than traditional methods for differential macroscopic constitutive models. Given the improved stability of the log-C transformation we propose a similar transformation to the Brownian configuration fields in the case of the FENE and FENE-P models.
In this presentation we will compare the stability of the usual BCF method with the log-based BCF method. Since for the FENE-P there exist a closed form differential constitutive equation, we will also study the stability and accuracy for the FENE-P model using three different methods: usual BCF, log-based BCF and log-C transformation.

[1] R. Fattal and R. Kupferman, JNNFM, 123 (2004) 281-285.
[2] M.A. Hulsen, R. Fattal and R. Kupferman, JNNFM, 127 (2005) 27-39.
[3] M.A. Hulsen, A.P.G. van Heel, B.H.A.A. van den Brule, JNNFM, 70 (1997) 255-261.

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A P3M Method for Computation of Many-Body Hydrodynamic Interactions in a Confined Geometry: Application to Migration and Apparent Slip in Nondilute Polymer Solutions

J. P. Hernandez-Ortiz, S. Anekal, M. D. Graham

University of Wisconsin, Madison, WI, USA

An O(N) particle-particle/particle-mesh method is presented for calculation of hydrodynamic interactions between N point particles in a confined geometry. This approach splits point forces into a local contribution for which rapidly-decaying free-space analytical solutions to the Stokes equations are used, and a global contribution whose effect is determined numerically on a mesh. A regularized point force solution is introduced, which mimics the behavior of the RPY tensor but is more amenable to the present computational scheme. The scheme is applied to Brownian dynamics simulations of flowing confined polymer solutions, and the effects of concentration on hydrodynamically-induced migration phenomena are illustrated. Preliminary results on an extension of the method including lubrication effects in a slit geometry are also presented.

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Frictional Drag Properties of Polymeric Solution in Complex
Kinematics Flows: A Multiscale Simulation Approach

Anantha P. Koppol [1], Rahdakrishna Sureshkumar [2],
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Modeling flow of dilute polymeric solutions in complex kinematics flows using closed form constitutive equations or single segment elastic dumbbell models has attracted considerable attention in the past decade. However, to date most simulations in complex kinematics flows have not been able to *quantitatively* describe the experimentally observed flow dynamics, such as vortex growth, free surface, interface motion etc., or the measured frictional drag properties [1-6]**.** This lack of quantitative prediction of experimental findings can be attributed to the fact that single segment elastic dumbbell models as well as closed form constitutive equations obtained by invoking various closures such as the FENE-P, FENE-LS can at best qualitatively describe the polymer dynamics and rheological properties of dilute polymer solutions as evinced by recent fluorescence microscopy studies of model macromolecules, namely DNA, in a variety of flow fields [7,8]. However, these studies have also demonstrated that multi-segment bead-rod and bead spring descriptions of dilute polymeric solutions can describe both single molecule dynamics such as molecular individualism, and unraveling dynamics, as well as the solution rheological properties such as viscosity and mean molecular extension with good accuracy [7,8]. These findings clearly underscore the fact that a multi-segment description of the macromolecule or reduced order coarse grained models that contain information regarding the internal degrees of freedom of the macromolecule are required for quantitatively accurate modeling of dilute polymer solutions under flow. Motivated by this fact, we have developed a highly accurate and CPU efficient algorithm for multiscale simulation of dilute polymeric solutions in complex kinematics flows using a bead-spring chains [9].

In this study, we have used our recently developed multiscale algorithm to model flow of a dilute polymeric solution through 4:1:4 axisymmetric contraction/expansion geometry utilizing single and multi-segment bead-spring descriptions as well as the FENE-P closed form constitutive equations. It should be noted that this geometry has been selected not only because it contains many important features of typical polymer processing flows, namely, contraction/expansion as well as recirculation but also due to the fact that a wealth of experimental data is available in terms of vortex dynamics and frictional drag properties [10,11]. In this presentation, we will discuss the influence of various model parameters, such as internal degrees of freedom, finite extensibility, closure approximation, and stress-conformation hysterisis on the predicted vortex dynamics and the frictional drag properties of the flow over a wide range of *De*. In turn, a unified approach for process level simulation of dynamics of dilute polymeric solutions will be suggested.

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DPD as a Tool for Rheological Characterization

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The rheology of dilute polymer solutions in simple shear and planar elongation flow is studied via computer simulation using the Dissipative Particle Dynamics (DPD) method. Polymers are modeled as bead spring chains with FENE springs. The implementations of DPD due to Spenley [SIAM J. Sci. Comput., 24, No. 4, 1267, (2003)] and Lowe [Europhys. Lett. 47 (2), 145, (1999)] are compared for these non-equilibrium flows. A secondary thermostatting method is introduced to remove the excess heat that evolves when flow is applied. Simple shear flow is modeled with Lees-Edwards boundary conditions, and planar elongational flow is implemented by using the boundary conditions developed by Kraynik and Reinelt [Int. J. Multiphase Flow 18, No. 6, 1045, (1992)], which were originally applied to non-equilibrium molecular dynamics studies. The time, length, and energy scales of DPD are self-contained, so we include a discussion of model parameter choice in order to match DPD polymers as closely as possible to physical systems for which experimental data are available.

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Atomistic Monte Carlo Simulation of a Polymer Melt under a Flow Field by Employing Generalized Ensembles

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We present a new simulation methodology which has a great potential for investigating the viscoelasticity of long-chain polymeric liquids, of relevance even to systems and conditions used in practical polymer processing operations. The main idea of the new scheme is to combine two different thermodynamically-founded simulation algorithms: GENERIC (General Equation for the Nonequilibrium Reversible-Irreversible Coupling) Monte Carlo (MC) [1,2,3] and Non-Equilibrium Molecular Dynamics (NEMD) [4]. With the new methodology, we are able to relate properly chosen state variables representing nonequilibrium states of the system of interest in the frame of the GENERIC formalism to the corresponding real, physical variables that directly bring about the same nonequilibrium states. We achieve this by taking first advantage of GENERIC MC to drive quickly the simulated system to certain nonequilibrium (but steady-) states of interest, and by performing next NEMD simulations to obtain all the important dynamical information of the nonequilibrium states. As a simple test case, we have applied the new scheme to a relatively short chain, linear polyethylene melt, and results will be presented for its response to a shear flow field. More importantly, it is expected that our new methodology (when properly incorporated within a coarse-grained modeling scheme) would make it possible to efficiently study the reptation regime of polymer melts.

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Rheological and Entanglement Characteristics of Linear Chain Polyethylene Liquids in Planar Couette and Planar Elongational Flows

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In this presentation, we compare and contrast the rheological and microstructural entanglement properties of a series of linear-chain polyethylene liquids under both planar Couette and planar elongational flow. We measure and compare the viscosities of the liquids in the two types of flow, and notice that both exhibit thinning behavior with increasing strain rate as the chains elongate and orient within the flow field. From the microstructural perspective, we examine the contributions of the chain energetics, such as bond-bending and bond-torsion, to the stress tensor and the degree of extension of the chains, as well as to the overall chain flexibility. Furthermore, entanglement characteristics, such as the shortest primitive path length, and the network configurations, are investigated--for the first time--as functions of strain rate in both vastly different flow fields. We expect the qualitative findings to be relevant to the understanding of entangled polymer melts, even though the available molecular weights are still below, or on the order of, the entanglement molecular weight.

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Transient 3D Flow of Polymer Solutions

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We have developed a versatile numerical method to simulate 3D transient flow of FENE polymer solutions, utilising a Lagrangian finite element mesh together with an adaptive remeshing scheme that includes Delaunay reconnection. The method extends the ideas of Harlen, Rallison, Szabo (J. Non-Newtonian Fluid Mech., 60 (1995) pp 81-104) to non-axisymmetric flows. We verify the method by application to the rheological benchmark problem of a spherical particle sedimenting axially in a cylindrical pipe. We then investigate the migration of a sphere positioned off-axis in a pipe.

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Steady Bubble Rise and Deformation in Bingham Fluids and Conditions for Their Entrapment

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We examine the buoyancy-driven rise of a bubble in a Bingham fluid assuming axial symmetry and steady flow. Bubble pressure and rise velocity are determined, respectively, by requiring that its volume and center of mass remain constant. The continuous constitutive model suggested by Papanastasiou is used to describe the viscoplastic behavior of the material. The flow equations are solved numerically using the mixed finite-element/Galerkin method. The nodal points of the computational mesh are determined solving a set of elliptic differential equations to follow the often large deformations of the bubble-surface. The accuracy of solutions is ascertained by mesh refinement and by predicting very accurately previous experimental and theoretical results for Newtonian fluids. We determine the bubble shape and velocity and the shape of the yield surfaces for a wide range of material properties. Besides the yield surface away from the bubble which surrounds it, unyielded material can arise either behind the bubble or around its equatorial plane in contact with the bubble. As the Bingham number increases, the yield surface at the equatorial plane and away from the bubble merge and the bubble gets entrapped. When the Bond number is small and the bubble cannot deform from spherical the critical Bingham number is 0.143, i.e. it coincides with the critical Bingham number for the entrapment of a solid sphere in a Bingham fluid. As the Bond number increases allowing the bubble to squeeze through the material easier, the critical Bingham number increases as well.

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Weakly Compressible Poiseuille Flows of a Bingham Fluid

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We solve the steady, creeping, weakly compressible plane and axisymmetric Poiseuille flows of a Herschel-Bulkley fluid. Under the assumption of weak compressibility, the pressure gradient is a function of the axial coordinate and satisfies a non-linear equation that involves the material parameters and the density of the fluid. The density is calculated by means of an equation of state. In the present work, both the linear and the exponential equations of state are considered. For a given pressure, the nonlinear equation can be solved using the Newton method and by means of numerical integration the pressure distribution can be calculated across the flow direction. The velocity profiles across the channel can then be constructed. It is shown that the position of the yield point approaches the wall as one moves upstream from the channel or capillary exit. As a result, for a given channel-length no flow can occur if the imposed pressure at the inlet is below a critical value.

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Numerical Simulation of Calendering of Viscoplastic Materials

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Numerical simulations have been undertaken for the process of calendering viscoplastic sheets with a finite thickness. The Finite Element Method (FEM) is used to provide numerical results for both cases of a fixed entry thickness or a fixed exit thickness under two-dimensional steady-state conditions. The Bingham-Papanastasiou model of viscoplasticity is used, which is valid for all ranges of deformation rates. Part of the solution is finding the separation point and the shape of the free surface of the exiting sheet. Yielded/unyielded regions are found *a posteriori* for a range of the dimensionless yield stress or Bingham number from the Newtonian limit (viscous fluid) to the fully plastic one (plastic solid). The 2-D FEM results show limited unyielded regions between the rolls, in disagreement with the Lubrication Approximation Theory (LAT), which predicts erroneous extended unyielded regions. However, LAT is very good at predicting the excess sheet thickness over the thickness at the nip, the pressure distribution and all engineering quantities of interest in calendering. Viscoplasticity leads to excess sheet thickness (at most 33% for extremely viscoplastic materials) as the dimensionless yield stress goes from zero (Newtonian behaviour) to one (plastic behaviour). All engineering quantities, given in a dimensionless form, increase substantially with the departure from the Newtonian values.

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Wave Evolution in Two-Layer Pressure Driven Flow - Newtonian Upper Layer over a Non-Newtonian Bottom Layer

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Purely fluid mechanical removal of a non-Newtonian (Herschel-Bulkley) soil layer by a laminar flow of a Newtonian cleaning fluid is simulated using level-set technique. The flow is two-dimensional, laminar, pressure-driven and two-phase (involves two liquids of different rheologies). Our simulations show the spatio-temporal evolution of the interface which is accompanied by shear thinning and consequent movement of the regions of the non-Newtonian layer near to the interface. Our results also show spontaneous development and growth of small amplitude interfacial waves to large-amplitude waves, leading to entrainment of the soil in the Newtonian cleaning fluid layer. The growth rates obtained from the numerical results will be compared against those obtained from an Orr-Sommerfeld type analysis of the full momentum conservation equations involving the non-Newtonian lower layer. These findings will be discussed in context of some previous and ongoing experimental observations.

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Squeeze Flow of Carbopol Gels

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Carbopol gels are viscoplastic materials that do not seem to have any elasticity. The squeeze flow test is a convenient method of measuring their yield stress. As a force is applied to a plate to squeeze the material, at a certain moment the movement of the plate stops and the material cannot be squeezed anymore. This finite height can be related to the yield stress of the material.
Experiments and simulations have been conducted for this type of squeeze flow with a constant force. The finite height is measured for different configurations and squeeze forces. The numerical simulations reveal interesting yielded/unyielded regions as the phenomenon progresses in time. Finally, a simple formula proposed by Covey and Stanmore in 1981 and based on the lubrication approximation, is applied to find the yield stress from the limiting height, and appears to give acceptable results.

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Blood Hemodynamics in Carotid Bifurcation: Influence of Rheological Models

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In this contribution, we investigate the behaviour of the pulsatile blood flow in a carotid bifurcation. The laminar and time dependent blood flow in a three-dimensional model corresponding to the carotid bifurcation is modelled by taking the advantage of finite volume method. Three-dimensional Navier-Stokes equations are coupled with three different constitutive equations: Newtonian, Carreau-Yasuda and Power law rheological model, last two describe the shear-thinning and inelastic behaviour of the human blood. The special attention is given to the influence of different rheological models for the blood flow on various hemodyamic factors. Here, we focus on those hemodynamic variables that are attributed to have the major role in initiation and development of atherosclerosis, e.g. low and/or oscillating wall shear stress, high pressure gradient, recirculation zones, etc.

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Using Newton-GMRES for Viscoelastic Flow Time-Steppers

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Kinetic theory models for polymeric liquids exhibit macroscopic dynamics that depend on a few, low-order moments of the underlying conformational distribution function. This dependence is generally exploited to write closed constitutive models for the stress tensor by assuming that the remaining higher-order moments quickly become functionals of these few, lower-order, slow moments. This occurs over timescales that are short compared to the timescale associated with the evolution of the slow moments.
Except for very simple kinetic theory models, this process entails the use of closure approximations for higher moments, and these closure approximations can have a significant, qualitative impact on model predictions. We present a method that avoids these approximations by exploiting the compact spectrum of eigenvalues exhibited by the linearized dynamical system. We take advantage of this spectrum of eigenvalues through Newton-GMRES iterations to enable dynamic viscoelastic simulators (time-steppers) to obtain stationary states and perform stability/bifurcation analysis.

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On a New Elastic Instability: Bifurcation in a Cross-Slot

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Very recently Arraatia et al. [Phys. Rev Letters Vol. 96(14) (2006)] demonstrated experimentally that the low-Re flow of a flexible polymer solution through a microfluidic “cross-slot” geometry can give rise to two different instabilities: a first instability in which the flow remains steady but is strongly asymmetric and a secondary instability in which the flow becomes unsteady and fluctuates non-periodically in time. Modelling the flow using a finite-volume technique we are able to show that both instabilities can be predicted using the Upper-Convected Maxwell model, thus demonstrating that this instability is purely elastic in nature. We find that the flow becomes asymmetric at a surprisingly low level of elasticity, around De=0.31 for the inertia-less case, and that this critical value displays very little sensitivity to mesh refinement. The effects of solvent viscosity, inertia and the use of more “realistic” models on the critical De will be discussed.

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Bifurcation Analysis of Flow Instabilities in Polymer Melts during Extrusion

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We use the concept of timesteppers [Kevrekidis et al., Comm. Math. Sciences, 1 (2003) 715] to perform systematic numerical bifurcation and stability analysis of a distributed-parameter model describing the dynamics of a plane Poiseuille flow of an Oldroyd-B fluid during extrusion with slip at the wall. In the past, it has been shown that due to the interplay between the nonmonotonicity of the slip equation and the viscoelasticity, the steady-state flow curve contains regimes with stable and unstable equilibria while self-sustained periodic oscillations appear when an unstable steady state is perturbed.
Here we further investigate the onset of such instabilities. We show for the first time that the loss of stability of steady-state solutions to sustained oscillating ones takes place through a subcritical Hopf bifurcation while the branch of stable periodic solutions loses stability through a critical point of limit cycles. This combination implicates the coexistence of stable steady states with stable and unstable periodic solutions in a narrow range of values of flow rates that can drive the system to abrupt loss of stability and under certain operating conditions to bursts.

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Modelling of Axisymmetric Instabilities Observed during the Electrospinning of Highly-Conducting, Non-Newtonian Jets

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Electrospinning is a novel process that allows the production of nanoscale fibres by using electrostatic force to accelerate a fluid jet. During electrospinning, it has been seen that axisymmetric instabilities can occur, giving rise to beaded fibres. In this paper we investigate these instabilities. Our model couples the laws of electrohydrodynamics with equations for polymeric rheological behaviour. A linear stability analysis is then performed which allows the unstable axisymmetric modes to be identified.

In this work we focus on the stability of solutions with high electrical conductivity such as PEO/water systems. Axisymmetric instabilities observed during electrospinning experiments have been captured using high-speed photography. The instability characteristics (growth rate, critical wavenumber) are extracted using image analysis, and the results are compared with the predictions from the theoretical model. The driving forces for instability are probed using an energy analysis.

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Cavity Filling Process Modeling by Rheological Characterization and Large Scale Computation

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Thermal cavity filling is at the heart of many polymer processes used to impart desirable surface structure on polymer items. Depending on the precise temperature-pressure history imposed, the produced item may not have the exact shape of the mold surface due to viscoelastic rebound in the pressure release stage. To minimize surface rebound, we developed a non-isothermal, viscoelastic free-surface flow model of the cavity filling process based on the DEVSSG-FEM. This novel model follows the polymer flow in the cavity through all process stages that traverse the polymer's glass transition. Although the model is two-dimensional, it applies a shape-dependent correction for three-dimensional flow effects on the polymer mass balance. Necessary parameters of the PTT rheological model employed are fitted from linear and nonlinear viscoelastic measurements and from direct process observables such as applied external force and total surface rebound. Due to the high computational requirements imposed by the multi-mode viscoelastic model and to the large number of cases that needed to be computed for parameter fitting, high-throuput computing on a network of distributed processors was employed. Results include thermal, stress and deformation field histories that showcase the model's predicting capability.

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A Parallel Adaptive Unstructured Finite Volume Method for Linear Stability (Normal Mode) Analysis of Viscoelastic Fluid Flows

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A parallel adaptive unstructured finite volume method is presented for analysis of the stability of two-dimensional steady Oldroyd-B fluid flows to small amplitude three-dimensional perturbations. A semi-staggered dilation-free finite volume discretization with Newton's method is used to compute steady base flows. The linear stability problem is treated as a generalized eigenvalue problem (GEVP) in which the right most eigenvalue determines the stability of the base flow. The eigenvalues corresponding to the right most eigenvalues associated with the most dangerous eigenfunctions are computed through the use of the shift-invert Arnoldi method. To avoid a fine meshing in the regions where the flow variables are changing slowly, an adaptive remeshing technique is used in order to increase numerical accuracy with a lower computational cost. The CUBIT mesh generation environment has been used to produce all quadrilateral unstructured meshes for a given mesh size function. In order to achieve higher performance on parallel machines the algebraic system of equations resulting from the steady and the generalized eigenvalue problems (GEVP) have been obtained by implementing the MUltifrontal Massively Parallel Solver (MUMPS). The proposed method is applied to the linear stability analysis of the flow of an Oldroyd-B fluid past through the linear periodic array of circular cylinders in a channel and the linear array of circular half cylinders placed on channels walls. The numerical results indicate good agreement with the numerical and experimental results available in the literature.

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A New Stability Mechanism Associated with the Oldroyd B Model in Creeping Flow Regime

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I will introduce a model closely related to the inertia-less Oldroyd-B model. The objective is to better understand the nonlinear coupling between the stress and velocity fields in viscoelastic flows, and thus gain insight into the reasons that cause the loss of accuracy of numerical computations at high Weissenberg number. The model is obtained by discarding the stress-advection and stress-relaxation terms in the Oldroyd-B model. The reduced (unphysical) model, which bears some resemblance to a viscoelastic solid, only retains the stretching of the stress due to velocity gradients and the induction of velocity by the stress field. The conjecture is that such a system always evolves toward an equilibrium in which the stress builds up such to cancel the external forces. This conjecture is supported by numerous simulations. This stability mechanism is however very subtle. In particular, the equilibrium manifold may have regions that are locally unstable, leading to a "peaking" behavior, in which solutions are initially repelled from the equilibrium manifold, but are eventually attracted back toward a stable equilibrium point on the same manifold. I will argue that a full resolution of this stability mechanism may pave the way toward a global-in-time existence theory.

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Coil-Stretch Transition and the Break Down of Continuum Models

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The breakdown of finite element (FEM) computations for the flow of an Oldroyd-B fluid around a cylinder confined between parallel plates, at Weissenberg numbers Wi = O(1), is shown to arise due to a coil-stretch transition experienced by polymer molecules traveling along the centerline, in the wake of the cylinder. With increasing Wi, the coil-stretch transition leads to an unbounded growth in the stress maximum in the cylinder wake. Finite element computations for a FENE-P fluid reveal that, although polymer molecules undergo a coil-stretch transition in the cylinder wake, the mean extension of the molecules saturates to a value close to the fully extended length, leading to bounded stresses with increasing Wi. The existence of a coil-stretch transition has been deduced by examining the behavior of ultra-dilute Oldroyd-B and FENE-P fluids. In this case, the solution along the centerline in the cylinder wake can be obtained exactly since the velocity field is uncoupled from the stress and conformation tensor fields. Estimation of the number of finite elements required to achieve convergence reveals the in-feasibility of obtaining solutions for the Oldroyd-B model for Wi > 1.

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On Kinetic Models for Dilute Suspensions of Rigid Rods

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We discuss the existence theory for certain kinetic models for the modeling of dilute suspensions of rigid rods. The model consists of a coupled Smoluchowski equation describing the evolution of a micro-scale together with Stokes flow for the motion of the solvent. For certain parameter values, the velocity gradient versus stress relation defined by the stationary and homogeneous flow is not rank-one monotone. We consider the evolution of possibly large perturbations of stationary flows and prove that, even in absence of a microscopic cut-off, discontinuities in the velocity gradient cannot occur in finite time.

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On the Gas Penetration in Periodically Constricted Circular Tubes Filled with Viscoelastic Liquids

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We examine numerically the displacement of viscoelastic liquids by pressurized air from harmonically undulated tubes of finite length. This unsteady process gives rise to a long open bubble of varying radius, increasing length and surrounded by the liquid. The viscoelastic part of the liquid stresses is subject to either the exponential PTT or the Oldroyd-B constitutive law. In general, the thickness of the liquid film that remains on the tube wall is non-uniform. Under creeping flow conditions, it varies periodically, but with a phase difference from the tube radius. The liquid fraction remaining in each periodic segment of the tube increases as the ratio between the minimum and maximum of the tube radius, decreases, whereas it tends to an asymptotic value for straight tubes, as the wavelength of the tube undulation increases, although here the flow is accelerating. The liquid fraction also depends strongly on the solvent viscosity and the exponential parameter of the PTT model. It increases as any of the two parameters decreases and tends to the Newtonian limit as takes large enough values. At high values of the Reynolds number, the film thickness increases with the axial distance, and the periodicity of the velocity and stress fields ahead of the bubble tip, which exists under creeping flow conditions, is broken. At even higher Reynolds numbers, recirculating vortices develop inside each tube expansion and when also decreases significantly, nearly isolated bubbles are formed in each tube segment, while the free surface exhibits corrugations.

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The log-Conformation Tensor Approach in the FVM Framework: Benchmark Solutions and Stability Analysis

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The log-conformation formulation proposed by Fattal and Kupferman [JNNFM vol.123, p.281 (2004)] has helped in providing further insights into the High-Weissenberg Number Problem. In this work we investigate the behaviour of that formulation within the Finite Volume Method (FVM) framework, by simulating several benchmark creeping flows of viscoelastic fluids: steady and unsteady flow through a 4:1 abrupt contraction, flow around a confined cylinder and flow through 4:1 square-square 3D abrupt contraction. Three models (UCM, Oldroyd-B and PTT) were used to assess the effect of different rheological behaviour on the flow patterns and solution stability. The polymer stress was calculated using both the standard and the log-conformation methodologies. For all test cases, the log-conformation technique provides solutions with similar accuracy as the standard approach when both methods converge to a steady solution. In terms of stability the log-conformation formulation is found to be much more robust with solutions achieved at very high Deborah numbers, although in some cases elastic instabilities do emerge.

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Oscillating Channel Flows of UCM and Oldroyd-B Fluids: Numerical and Analytical Solutions

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Time dependent simulations of viscoelastic flows are becoming more and more frequent, not only because many of the flows of interest in engineering and other applications such as biomechanics are inherently unsteady, but also due to the fact that elastic instabilities tend to develop in apparently steady flows. It would be useful to have some relatively simple test cases involving unsteadiness, preferably possessing analytical solutions, for the purpose of assessing general numerical codes which are usually designed for rather more complex situations. A new test case is here proposed and the corresponding analytical solution obtained: a periodic flow in a long channel resulting from the application of a sinusoidal pressure gradient. It offers some advantages over the more classical startup flow employed in many recent studies involving UCM and Oldroyd-B fluids. It is a periodic, rather than transient, flow and thus less sensitive to the exact initial conditions. Unlike the UCM startup case, it does not involve discontinuities in gradients which lead to localized numerical wiggles. Yet, this simple 1D periodic flow is a hard test case, as it will be shown.

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Numerical Simulation of the Flow of a PTT Fluid past a Cylinder

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The unsteady two-dimensional viscoelastic flow of a simplified exponential Phan-Thien Tanner fluid (S-PTT) past a non-confined cylinder is simulated. The Elastic Viscous Split Stresses (EVSS) formulation is used to decompose the extra-stress tensor to enhance the stability of computations. The governing equations are written in generalized orthogonal coordinates and the finite volume method used to solve them. The QUICK scheme is employed to evaluate advection, whereas diffusion and curvature terms are approximated with centered formulas. For time marching, diffusion, advection and acceleration terms are treated explicitly and pressure implicitly to enforce mass conservation. The overall formulation is second order accurate in space and first order accurate in time.
The code is validated for Newtonian flow, confirming that the onset of von Karman instabilities occurs at Reynolds number Re = 47. The viscoelastic calculations up to Deborah numbers 1.5, show that the onset of instabilities appears at Reynolds numbers higher than that of the Newtonian case. Results for the drag coefficient and Strouhal number will also be commented.

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On the Numerical Treatment of Integral Models for Elasticity in a Compressible Fluid

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The incorporation of elasticity into a compressible fluid has involved a revisitation of the principle of objectivity in constitutive relations. Using techniques from differential geometry, we verify that it is essential to work with the relative left Cauchy-Green tensor (and not the relative right Cauchy-Green tensor). It is important to go back to first principles here because compressibility alters some of the relations in current use, e.g. the relative left Cauchy-Green tensor should appear in the integrand with relative density. Elasticity is most easily explored using the Oldroyd B or other differential constitutive equations for the stress tensor. All differential models have an equivalent explicit integral relation for stress involving the metric tensor and its convected derivatives. Integral relations are capable of generalising differential models. Models such as K-BKZ probably have no exact differential equivalent. Recently, these integral relations have been numerically explored using finite elements over time. Typically the integrand contains a time-varying matrix representing the relative left Cauchy-Green tensor, which considerably distorts over a relatively short period of time. This matrix is typically multiplied by an exponentially decaying function so that after a certain period of time the integrand becomes negligible. We modify a technique used in Peters et al. (2000), which solves for the relative left Cauchy-Green tensor at each time step and sums the contributions. We introduce a new idea, which involves direct solution procedure for an object that decreases in size the further forward in time it progresses, thus giving greater control and reliability. This approach has been incorporated into the journal bearing problem and initial results suggest a significant effect of elasticity on journal bearing stability. For testing purposes, we have at present only incorporated Oldroyd B as an integral relation but the structure is in place for easy implementation of more complex integral models.

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Viscoelastic Analysis of Complex Flows: From the Constitutive Model through the Numerical Simulations and their Experimental Validation

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In this work we present some interesting results (i.e., helical flow and big vortices) concerning the viscoelastic behavior of branched polymer melts in 3D complex flow conditions. Most of the studied 3D geometries are natural generalizations of the 2D classical benchmark flow problems, like the planar contraction flow or the pressure-driven cavity flow. The Single-equation version of the eXtended Pom-Pom (S-XPP) model is implemented to describe correctly the complex rheology of branched polymers. The numerical results are compared with the experimental data in terms of flow kinematics and stress distribution characterized by flow-induced birefringence.
The main conclusion concerning the constitutive model is that although mathematically equivalent, not all the versions could be implemented efficiently in numerical flow analysis, especially in the presence of geometrical singularities. Our study clearly shows that a full 3D analysis in combination with an efficient constitutive model are definitely required for describing correctly the flow behavior under different experimental flow conditions.

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Numerical Simulation of Viscoelastic Flows in Cross-Slot Flow Devices

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Cross-slot flow is investigated through a mixed finite element/finite volume algorithm, employing sub-cell discretisation for stress with cell-vertex finite volume technology. In contrast to contraction flows, here the steady problem manifests strong flow features through the long-time exposure to significant extension. Solutions are compared and contrasted for a range of rheological models of varying shear and extensional response. This includes phenomenological-based models from network-theory of Oldroyd/Phan-Thien-Tanner class, and also the kinetic-theory based pom-pom models. Force-driven flow, as opposed to flow-rate driven, is adopted for generality and to accurately represent boundary conditions. Match is sought on peak extensional viscosity and Trouton ratio behaviour. The consequence of severe strain-hardening is made apparent under Oldroyd modelling, and trends in velocity fields and principal stress difference are evaluated for increasingly elastic fluids.

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Prediction of Die Swell in Polymer Melt Extrusion Using an Arbitrary Lagrangian Eulerian (ALE) Based Finite Element Method

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Accurate prediction of die swell in polymer melt extrusion is important as this helps in appropriate die design for profile extrusion applications. Die swell prediction has shown significant difficulties due to two key reasons. The first is the appropriate representation of the constitutive behavior of the polymer melt. The second is regarding the simulation of the free surface, which requires special techniques in the traditionally used Eulerian framework. In this paper we propose a method for simulation of die swell using an Arbitrary Lagrangian Eulerian (ALE) technique based finite element formulation. The ALE technique provides advantages of both Lagrangian and Eulerian frameworks by allowing the computational mesh to move in an arbitrary manner, independent of the material motion. In the present method, a fractional step ALE technique is employed in which the Lagrangian phase of material motion and convection arising out of mesh motion are decoupled. In the first step the relevant flow and constitutive equations are solved in Lagrangian framework. The simpler representation of polymer constitutive equations in a Lagrangian framework avoids the difficulties associated with convective terms thereby resulting in a robust numerical formulation. In the second step, mesh is moved in ALE mode and the associated convection of the stress due to relative motion of the mesh is performed using a Godunov type scheme. While the mesh is fixed in space in the die region, the nodal points of the mesh in the extrudate region are allowed to move normal to flow direction with special rules. A differential exponential Phan Thien Tanner (PTT) model is used to represent the constitutive behavior of the melt. Using this method we simulate die swell in planar and axisymmetric extrusion with abrupt contraction ahead of the die exit. This geometry allows the extrudate to have significant memory for shorter die lengths and acts as a good test for swell predictions. We demonstrate that our predictions of die swell match well with reported experimental and numerical simulations.

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Non-Isothermal Simulation of the Film Blowing Process Using a Multi-Mode Extended Pom-Pom Model

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Plastic films are largely produced using film blowing process. Branched polymers such as LDPE are commonly used in this process to produce variety of plastic films. In this study, recently developed eXtended Pom-Pom (XPP) model which focuses on describing rheological behavior of the branched polymers is employed to analyze the non-isothermal flow in the film blowing process. Furthermore, Nakamura equation for crystallization kinetics is employed to consider crystallization effects and improve prediction of the state of the stress in the film. Results of the numerical analysis show very good agreement with the reported experimental data. Predictions for the strain rates in machine and hoop directions which are critical for the estimation of the stress are also compared with the reported data and showed reasonably good agreement.

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Computing with Power-Law Viscoelastic Materials

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Commonly many viscoelastic computations proceed with only a single relaxation mode, and flow is steady. Removal of these restrictions often creates problems in computing. An extreme example has been found in attempts to compute the recoil of soft solids. For example, the description of the recoil of bread dough needs either a continuous power-law relaxation spectrum, or at least 14-16 discrete modes as an approximation. The response varies from a millisecond to 1000 seconds. We report our attempts to compute this response and a comparison with experiments.

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Characterization of the Compressive Behaviour of Brain Tissue and Constitutive Modelling

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Of all body parts, the head is the most vulnerable part and is often involved in life-threatening injury. Each year, a total of 90 thousand fatalities occur as a result of traumatic brain injury (TBI) and almost 4.7 million people sustain a TBI each year in the United States and the European Union.
To predict the mechanical response of the contents of the head during impact, Finite Element (FE) models are employed. They contain a detailed geometrical description of anatomical components but lack accurate descriptions of the mechanical behaviour of the brain tissue. The mechanical properties of brain tissue have been studied for 50 years, however no universally accepted data exists that describes its viscoelastic behaviour, in particular in multiple deformation modes.
The objective of this work is to obtain a data set describing the non-linear viscoelastic response of brain tissue in different deformation modes and to validate a previously developed constitutive model. The large strain stress relaxation response is determined for porcine brain samples in both shear and compression. Different compression protocols are evaluated showing the importance of choosing the proper experimental conditions. Compression measurements with and without initial contact between the sample and a teflon-coated plate are compared. The influence of a fluid layer surrounding the sample and the effect of friction are examined and show an important role during compression measurements. Moreover, the hypothesised reason for the effect of the experimental conditions is confirmed by model simulations.
A non-linear viscoelastic constitutive model that was developed based on large shear stress relaxation measurements has previously shown good predictions up to 50% shear strain. In this paper, the ability of the model to describe the behaviour in other deformation modes is assessed using stress relaxation results up to 20% compressive strain of 35 porcine brain tissue samples. In addition to the compressive response, also the tensile behaviour remains to be investigated. Furthermore, anisotropy and regional differences can play an important role in the mechanical behaviour of brain tissue. The model has been implemented in the explicit FE code MADYMO. Simulations with a 3-D head model using the new constitutive model were compared with predictions using a linear viscoelastic model and the model developed in Brands et al. (J. Biomech., 2004).

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Experimental and Numerical Evaluation of Drop Deformation and Break-up in Complex Flow Fields

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Studies on disperse systems undergoing flow are often based on single drop measurements carried out in simple shear or pure elongation. The flow present in actual process equipment is, however, usually very complex. We therefore have carried out single drop experiments in a complex flow field generated by a rotor-stator device. The setup consists of two concentric cylinders with 6 teeth on each cylinder wall. The cylinder gap is filled with the continuous liquid phase and as the cylinders are rotated in opposite directions a complex flow field is generated. During an experiment the drop position and drop deformation are monitored using digital cameras. Post-processing of the image data leads to the particle track and deformation history of the drop.
We have also developed a 3D code which can describe the deformation and break-up of drops in Stokes flows. The discretization of the flow field is carried out using finite elements while the interface is tracked using the Volume of Fluid (VOF) method. Interfacial tension is included using the Continuous Surface Stress (CSS) formulation. For a given experiment in the rotor-stator device the local flow field is calculated along the particle track. This is then used as input for the 3D finite element/VOF code in order to generate a flow field similar to the one experienced by the drop. Comparison between numerically and experimentally obtained drop deformations is hereafter made.

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Experimental and Numerical Study of Cavitation in Journal Bearings

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During the flow of oil within a dynamically-loaded journal bearing, the lubricant may experience wide ranges of temperature and pressure. In such a situation, the effective tensile strength of oil is an important consideration in the assessment of flow boundary conditions within fluid film bearings, their load bearing capacity and the cavitation damage potential of liquids. The term "cavitation" usually refers to the formation of bubbles in a liquid when it experiences "negative pressure" or tension. If the tension exceeds a liquid's cavitation threshold or effective tensile strength, F_c, at that temperature it changes irreversibly into a two-phase system of liquid and a mixture of vapour and dissolved gas, the latter appearing as cavitation bubbles. The subambient pressures which give rise to cavitation in lubricating films may be either gaseous or vaporous: the former may arise due to ventilation from the surrounding atmosphere, or by the dissolution of gases, whereas vaporous cavitation results if the pressure in a lubricant falls to (or below) its vapour pressure. It is the latter phenomenon, which is the subject of the present paper. Homogeneous nucleation theory predicts that the formation of vapour bubbles requires large tensions, some 1.3 kbar for water. Cavitation in common engineering liquids such as lubricants usually involves heterogeneous nucleation at lower tensions and, in the absence of an adequate theory, it is necessary to measure the cavitation threshold of such liquids. To be of engineering relevance, such measurements (which are necessarily of the liquid's "effective" tensile strength) must be made under pertinent conditions. These can involve enormous rates of negative pressure development (>1 bar/^{o}C-s) and a wide range of temperatures (up to 150^{o}C in the case of some motor oils). We report measurements of the effective tensile strength, F_c, of commercial "multigrade" oils (in the SAE viscosity grades 5W-30 and 10W-40) over a range of temperatures, T, which are representative of those encountered under their normal operating conditions (in the range $20^oC < T < 140^oC$). Also reported are the values of F_c which are obtained for Newtonian silicone oils over a range of shear viscosities. In the experiments reported herein, samples of liquid are subjected to dynamic stressing by a pressure-tension cycle, this being a feature of the conditions experienced by a lubricant within a dynamically-loaded journal bearing and the method used to estimate F_c avoids reliance upon direct measurements of substantial dynamic tensions using conventional pressure transducers. In our previous work, we have modelled cavitation in a lubricant using a single-phase incompressible model in which the cavitation region is modelled by allocating a low viscosity to the fluid in this region. The effect of this is to rapidly decrease the viscosity in this region. In the present study, a compressible viscous isothermal model is presented for journal bearing lubrication. The viscosity in the model thins with decreasing density. The governing equations are written in terms of velocity, the natural logarithm of the density and the kinematic extra-stress tensor. A semi-Lagrangian treatment of the material derivatives is combined with a spectral element discretization in space. The roles of the speed of sound and the eccentricity ratio on the load bearing capacity of the journal bearing are investigated. Compressibility is shown to enhance the load bearing capacity and this effect is amplified as the eccentricity ratio approaches unity. It is shown that for speeds of sound in the region of those of multigrade oils, the dominant component of the force on the journal acts along the line joining the centres of the bearing and journal and in the direction away from the narrow gap.

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Modeling of Nonisothermal Electrospinning of Polymer Melts with and without Crystallization

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In electrospinning, applied electric field elongates a charged fluid jet to produce nanofibers. Polymer melts can be electrospun nonisothermally, which is environmentally benign and economically attractive. We present a nonisothermal thin-filament model for the stable jet region of electrically-driven free-surface viscoelastic flow. The traditional asymptotic thinning is replaced with a new boundary condition to account for low inertia in highly viscous viscoelastic jets. Numerical solutions for various experimental conditions agree with digitized images of polylactic acid melt jet near the spinneret and the final jet sizes from experiments where whipping motion was suppressed by rapid cooling. Some polymers such as nylon can crystallize in-flight, and thus a simple crystallization model is incorporated. To account for coupling of the highly elongational flow with crystal morphology evolution, a mesoscale approach has been developed and preliminary results will be presented.

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Structure-Property-Relationships for the Newtonian and the Non-Newtonian Flow of Polymer Solutions

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The flow behavior of polymer solutions in the Newtonian region is important for many technical applications and has already been described for a broad range of different systems in earlier publications. Although the viscosity of a polymer solution depends on many effects, like molar mass and the chemical structure of the polymer, concentration, temperature, shear rate and the chosen solvent, it can be estimated via a simple viral equation.
Since the critical shear-rate of polymer solutions is exceeded in many technical processes, the knowledge of the non-Newtonian flow behavior is important. In the Non-Newtonian region the elastic properties of fluids, represented by the first Normal-Stress-Difference N_1 become more dominant.
We present a detailed report of rheological and polymer analytical investigations of various polymer systems of synthetic and biologic origin. Based on the structural information the Newtonian and the non-Newtonian material functions in shear and oscillation of polystyrene standards and water soluble biopolymers depending on molar mass, concentration, solvent quality, temperature and shear rate are presented and discussed.

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Dynamic K-L Analysis of Coherent Structures Based on DNS of Turbulent Newtonian and Viscoelastic Flows

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The turbulent dynamics corresponding to Direct Numerical Simulation (DNS) data of Newtonian and viscoelastic turbulent channel flows is analyzed here through a projection of the velocity fields into a set of Karhunen-Loeve (K-L) modes, large enough to contain, on the average, more than 90% of the fluctuating turbulence energy.
Previous static K-L analyses have demonstrated a dramatic decrease in the K-L dimensionality (and, correspondingly, the number of modes carrying most of the turbulent energy) accompanying the presence of viscoelasticity in turbulent channel flows; this is consistent to the increasing importance of large coherent structures for viscoelastic turbulent flows, as also has been revealed in flow visualizations of DNS data. We exploit this feature here in using the K-L modes dynamically to gain quantitative insights into the behavior of the overall flow dynamics, which may eventually help to explore approaches towards a low-dimensional modeling of the viscoelastic turbulence.
A representational entropy constructed from the projection coefficients is used in conjugation to the calculation of the fluctuating kinetic energy to provide additional evidence that viscoelastic turbulent flow is better organized than in the Newtonian limit. Moreover, dynamic correlation analysis between pairs of K-L coefficients showed a systematic increase in the time scales characterizing dynamic turbulent events with viscoelasticity. These correlations have distinct pulse behavior characteristic of intermittence and quasi-periodicity in turbulence.

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A log-Exponential Mapping for the Preservation of Positive Definiteness in the Numerical Integration of Viscoelastic Constitutive Models

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We present a new method in order to integrate the evolution equation for a symmetric and positive definiteness second order tensor (SPD) which results when modeling the transient flow behavior of viscoelastic fluids. The method is based on the log-conformation representation, also reported earlier by Fattal & Kuprferman, JNNFM 2004 & 2005, the application of the Cayley-Hamilton theorem for second order tensors and an additional mapping which ensures that the tensor remains always bounded. The algorithm is used for the simulations of viscoelastic turbulent channel flow, which have been received great attention since mid 90's with ultimate goal to enlighten the phenomenon of maximum drag reduction usually observed in wall bounded flows. The main new feature for the implementation of the proposed scheme is relied on a second order finite difference multigrid diffusion which guarantees the positive definiteness of the conformation tensor. Sample results will demonstrate the window of parameters where the new algorithm can prove to be of uselfulness to numerical simulations of viscoelastic turbulent flow.

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Direct and Large Eddy Numerical Simulations of FENE-P Drag Reduction Flows

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We report on numerical simulations of the turbulent channel flow of a dilute polymer solution modeled with the FENE-P constitutive equation. The computations are based on a time-splitting algorithm and a hybrid spectral-finite difference spatial discretization. Direct numerical simulations (DNS) are first considered at a friction Reynolds number 180 for molecular extensibilities spanning the low and high drag reducing regimes. Then a new temporal large eddy simulation (TLES) is applied on a coarse grid. A temporal approximate deconvolution method (Pruett et al., Phys. Fluids, 18, 2006) is used to model the Newtonian turbulent subfilter stresses. Results are presented for TLES with and without subfilter modeling of the conformation tensor equations. These show that TLES tends to underestimate drag reduction, but with the predictive capability of the TLES improving with secondary regularization in the conformation tensor equation.

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A Turbulence Closure for Viscoelastic Fluids Based on the FENE-P Model

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DNS research on turbulent channel flow of FENE-P fluids has provided data at high enough Reynolds numbers to allow the development of closures for RANS type equations, such as zeroth-order model of Li et al (JNNFM 140 (2007) 177). For industrial applications higher order turbulence closures are required and further developments needed.
A low Reynolds number *k*- turbulence closure for FENE-P fluids is developed based on DNS data for low drag reduction in channel flow (*Re* = 395, *We*□= 25, = 0.9, L^2= 900). Closures are provided for the new viscoelastic stress power (work done by viscoelastic stresses) and turbulent transport terms as well as to the non-linear turbulent term (NLT) arising in the rheological constitutive equation and comparisons are made with the corresponding DNS data. The model for the viscoelastic stress power relies on an accurate modeling for NLT, whereas the viscoelastic turbulent transport term is of less relevance in the transport equation of *k*.
Predictions of fully-developed channel flow are carried out after adaptation of a boundary-layer code. The results show the potential of this approach and indicate routes for further model development.

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DNS Experiments of Surfactant Drag Reducing Fluid Flows

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Drag reduction by additives is a physical phenomenon, which induces a significant reduction of friction under a turbulent flow. The additives responsible for this phenomenon are fibres, polymers and surfactants in solution.

Except for the fibres, the additives are introduced as simple monomers or molecules into the solvent. Then, an aggregation process leads to the generation of macromolecules or micelles. All the aggregates or particles responsible for the Drag reduction have got a huge aspect ratio. They are flexible, elastic and are rather small in comparison for the size of the pipe.

Several assumptions were made to explain this phenomenon such as the orientation of the particles with the flow. Extensional viscosity and viscoelasticity are found to play an important role. It seems, following several DNS's works (Sureshkumar et al. [1], Beris and Dimitropoulos [2], Dimitropoulos et al. [3], De Angelis et al. [4], Housiadas and Beris [5], ...), that viscoelasticity is the major parameter in the case of polymer solutions. And the best representation for such a Drag Reducing solution seems to be the FENEP model.

In the case of surfactant solutions, the effect of viscoelasticity is not always of evidence. Thus, Lu et al. [6] showed that some drag reducing surfactant systems were not viscoelastic. Particularly, the Shear Induced Structure, which is associated with a local increase of the viscosity (Shear-thickening), seems to play an important role in the modification of turbulence properties studied. So we explored by DNS a simple law representing a shear-thickening behaviour (Guillou and Makhloufi [7]). From our results it appears that this law based on a viscous model can not fit the friction coefficient behaviour obtained experimentally. So, this model can not explain the phenomenon. These results ask some questions about drag reducing solutions which are not viscoelastic. Some of our experiment (Hadri et al. [8]) showed the presence of sliding at the wall. This may be a way for an explanation.

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POSTER CONTRIBUTIONS

A Generalized Single-Conformation Tensor Viscoelastic Model Based on Principles of Non-Equilibrium Thermodynamics

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Guided by the GENERIC and bracket formalisms of non-equilibrium thermodynamics [1,2], we present a generalized single-conformation tensor based viscoelastic model which reduces to known rheological models, such as the Giesekus, the Phan-Thien/Tanner and the FENE-P ones, under certain limiting conditions. The new model incorporates the dissipation or friction matrix corresponding to the Giesekus model but, in addition, accounts for finite-extensibility effects as well as for anisotropic effects in the relaxation spectrum in the spirit of the White-Metzner model. Key in the new model are two functions: the free energy function (associated with the elasticity of the fluid) and the friction matrix (associated with dissipation effects). In essence, the new model extends or corrects the Giesekus model to account for the finite extensibility of the chain at high deformation levels. We will present the predictions of the model in the simple shear and 1D-extensional flows, we will discuss its capability to fit available rheological data for a number of polymers, and we will comment on the opportunity it offers to accommodate within the constitutive equation more complicated, bounded expressions for the free energy of the deformed liquid such as those proposed for highly elastic materials.

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Numerical Simulation of Complex Fluid Flows with Non-Newtonian Differential Models

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This paper deals with the numerical simulation of three-dimensional isothermal fluid flows of polymeric melt materials. In order to describe the measured visco-elastic material behavior of polycarbonate at melt temperature we use models of a differential type. The numerical simulation is accomplished with a commercial finite volume program which is upgraded by transport functions for the additional extra stress components. These differential equations have to be solved simultaneously with the equations of the fluid flow. For simple geometries we analyze the accuracy and the limits of the numerical calculations in comparison with analytic results respectively literature. Finally the fluid flows in complex geometries like single and twin screw extruder are investigated. The results show the influence of the visco-elastic properties to the fluid flow in contrast to a fluid with the same non-linear yielding without elasticity.

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Numerical Simulations of Flow in a Variable-Speed Corotating Twin Screw Extruder

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The flow field and mixing pattern in a variable speed corotating intermeshing twin-screw extruder is studied. In this extruder, the two screws have different number of flights and rotate at different speeds. Results from numerical simulations and flow visualization experiments suggest that this extruder exhibits superior distributive mixing in comparison with a regular corotatingg twin-screw in which the screws are identical and rotate at the same speed. In addition, this new screw design exhibits a more positive flow displacement action and a shorter average residence time.

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Correlating the Rheology of PVC Pastes with Particle Characteristics

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Plastisols are mixtures of PVC particles dispersed in a continuous phase, the plasticizer. For an adequate application of the plastisol its rheology has to be closely controlled. Furthermore, PVC pastes exhibit a complex rheological behaviour, strongly dependent on the particle characteristics, and which changes with ageing time.
The present study was aimed at identifying which particle characteristics (size and size distribution, porosity and surface characteristics) most affect the rheologial behaviour of the pastes. So far, we have fixed the particles composition (PVC of constant molecular weight) and the plasticizer (DIDP- Di-Isodecyl Phthalate).
The ultimate objective is to model the reology of PVC pastes as a function of particle characteristics. This requires good experimental data to support the modelling. Thus, to this point, we have directed our attention to the development of an experimental strategy to produce such data. A systematic rheological characterization of PVC pastes, both flow and dynamic tests, was performed and, simultaneously, the size distribution of the aggregates in the plastisols was followed using a laser diffraction technique (LDS). This required the development of a methodology to enable the use of LDS to measure the size distribution of the aggregates in the concentrated paste. Tests were performed for different ageing times.
In this study we have varied the size distribution of the PVC latex used to form the dry aggregates and the surface characteristics of the latex and thus of the aggregate. Particles (aggregates) with different size distributions, porosity and surface characteristics were used in the experimental tests.
The results obtained so far, show that changing these variables affects not only the initial rheological behaviour of the plastisols, but also the ageing process of the paste (strength of the aggregates varies with time and is dependent on the aforementioned parameters).

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Rheological Characterization of Foodstuff Used in Rolling Experiments and Modeling via Integral Constitutive Equations

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The calendering and rolling processes are used in a wide variety of industries for the production of rolled sheets or films of specific thickness and final appearance. The acquired final sheet thickness depends mainly on the rheological properties of the material. Materials which have been used in the present study are foodstuff (such as mozzarella cheese and flour-water dough) used in food processing. These materials are rheologically viscoplastic-elastic. They have been rheologically characterized using a parallel-plate, an extensional, and a capillary rheometer at room temperature. Based on the linear and non-linear viscoelastic and viscoplastic data, two constitutive equations have been formulated, namely a viscoplastic Herschel-Bulkley model and a visco-elasto-plastic K-BKZ model with a yield stress. For cases where time effects are unimportant, the viscoplastic Herschel-Bulkley model can be used. For cases where transient effects are important, it is more appropriate to use the K-BKZ model with the addition of a yield stress. Finally, the wall slip behaviour of dough was studied in capillary flow, and an appropriate slip law was formulated. These models adequately characterize the rheological behaviour of bread dough and constitute the basic ingredients for flow simulation of dough processing, such as extrusion, calendering and rolling.

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Predicting the Behaviour of Nylon-6 through Industrial Spin Packs

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In fiber spinning of polyamide-6 (nylon), the spin pack is equipped with a range of wire-mesh filters through which the melt must pass to become fine fibers. The problem of the prediction of the fluid dynamics pattern through wire-mesh filters is akin to flow through porous media, where Darcy's law may be used to predict the pressure drop vs. flow rate of the system. Experiments of a Newtonian silicone oil and polyamide-6 have been run in a pilot-plant equipment, and the pressure results are given for different wire-mesh filters. Then, fitting of the data with Darcy's law is carried out with the aim of finding the ratio K/H, where K is the permeability of the porous media and H is the height of the porous media. These values are then used for testing all experimental pressure drop data against the model predictions. Finally, pilot-plant results are given for spin-packs containing spinnerets, filters, and metal sand.

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Numerical Simulation of the Extrusion of Strongly Compressible Liquid Foams

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The axisymmetric and plane extrusion flows of a liquid foam are simulated assuming that the foam is a homogeneous compressible Newtonian fluid that slips along the walls. Compressibility effects are investigated using both a linear and an exponential equation of state. The numerical results confirm previous reports that the swelling of the extrudate decreases initially as the compressibility of the fluid is increased and then increases considerably. The latter increase is sharper in the case of the exponential equation of state. In the case of non-zero inertia, high compressibility was found to lead to a contraction of the extrudate after the initial expansion, similar to that observed experimentally with liquid foams, and to decaying oscillations of the extrudate surface. The time-dependent calculations show that the oscillatory steady-state solutions are stable. These steady-state oscillatory solutions are not affected by the length of the extrudate region nor by the boundary condition along the wall.

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Annular Poiseuille Flow of a Newtonian Liquid with Non-monotonic Slip along the Walls

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The Poiseuille flow of a compressible Newtonian fluid assuming that slip occurs along the wall is studied. Different slip models relating the wall shear stress to the slip velocity are employed. In the case of linear slip, it is easily shown that the slip velocity along the inner cylinder is always greater than the slip velocity along the outer cylinder. In the case of a non-monotonic slip equation, there exist linearly unstable steady-state solutions corresponding to the negative-slope regime of the slip equation. As a result, the resulting flow curve is also non-monotonic with an intermediate unstable negative-slope branch, which corresponds to the stick-slip extrusion instability regime. It is shown for small radii ratios $\kappa=R_1/R_2$, two stable steady-state solutions are possible in a certain range of the volumetric flow rate. As a consequence, the stick-slip instability regime is reduced in size and eventually disappears as κ is decreased. This provides an explanation for the fact that the stick-slip instability is not observed in annular extrusion experiments.

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Comparative Study on Multi-Mode Constitutive Equations for Film Blowing Process

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Film blowing process has been modeled for more than three decades. It involves extensional flow in different rates of deformations, therefore choosing an appropriate multi-mode viscoelastic equation is an important step in modeling and understanding of the process. In this study multi-mode PTT-a, and XPP models are implemented, and the results of the simulation for different spectrum of relaxation times are presented and compared. While both models are successful in predicting film blowing characteristics, there are significant differences in estimation of the deformation rates and stresses.

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The Temperature Dependence of the Rouse Mode Relaxation Spectrum and Zero Shear Rate Viscosity in Cis-1,4-Polybutadiene: Results from Long Atomistic Molecular Dynamics Simulations down to the Glass Transition Temperature T_g

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A well-relaxed atomistic configuration of a 32-chain C_{128} cis-1,4-polybutadiene (*cis*-1,4-PB) system has been subjected to long (on the order of a few microseconds) molecular dynamics (MD) simulations in the NPT ensemble using the united-atom forcefield introduced by Smith and Paul [1] on the basis of quantum chemistry calculations. This allowed us to study in detail the temperature dependence of the Rouse-mode relaxation spectrum of *cis*-1,4-PB over a wide range of temperature (from T=430K down to 165K) and pressures (from P=1 atm up to P=3.5 kbar) conditions. Results are presented here for: (a) the time decay of the autocorrelation function of the normal coordinates (Rouse modes), (b) the single chain intermediate coherent dynamic structure factor, $S_{coh}(q,t)$, and (c) the intermediate incoherent dynamic structure factor, $S_{inc}(q,t)$, for different values of the wavevector q. By mapping our MD simulation results onto the Rouse model, we have also been able [2] to extract a prediction for the zero shear rate viscosity of the simulated cis-1,4-PB system as a function of temperature (for temperatures as low as down to T_g) and compute its fragility index.

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