IWNMNNF 2023

21st International Workshop on Numerical Methods for Non-Newtonian Flows

Lodge on Loch Lomond, Luss, Scotland

29 May - 1 June 2023

Organisers:

Mónica S. N. Oliveira, University of Strathclyde
Konstantinos Zografos, University of Strathclyde
Robert J. Poole, University of Liverpool
Marco Ellero, Basque Center for Applied Mathematics
Patrick D. Anderson, Eindhoven University of Technology

Tuesday, 30^{th} May

Session 1: 8:50 am - 10:40 am

Welcome

Predicting the efficacy of foams in sclerothapy
Simon Cox, Tirion Roberts, Denny Vitasari

Modeling of multiphase displacement flow of foamed fluids in annular geometries
Rafael P. M. Moreira, Mônica F. Naccache

A Conservative Level-Set Method for Multiphase Viscoelastic Flows
W. Doherty, T. N. Phillips, Z. Xie

Enhancing the applicability of the elliptic grid methods for flow with moving boundaries
Pantelis Moschopoulos, Alexandros Spyridakis, Stylianos Varchanis, Yannis Dimakopoulos, John Tsamopoulos

Session 2: 11:05 am - 12:45 pm

The rheology of non-Brownian suspensions under inhomogeneous flow
Christopher Ness

Simulations of concentrated suspensions of rough polydisperse particles using tribological friction models
Jose A. Ruiz-Lopez, Sagaya S. Prasanna Kumar, Adolfo Vázquez-Quesada, Juan de Vicente

Scaling relations between viscosity and diffusivity in shear-thickening suspensions
Abhinendra Singh, Kuniyasu Saitoh

Particle redistribution in a horizontal Couette
Mahdi Davoodi, Andrew Clarke

Session 3: 2:00 pm - 3:40 pm

Complex viscoplastic flows in superhydrophobic channels: A modeling framework

Seyed Mohammad Taghavi, Hossein Rahmani

Synergy between elasticity and plasticity of the fluid in complex internal flows

Emad Chaparian

Thixo-viscoelastoplastic constitutive modelling using an elastic energy-dissipation measure and its validation in complex flow

J. Esteban López-Aguilar, Michelle Figueroa-Landeta, H.R.Tamaddon-Jahromi, Marco Ellero

Dynamical analysis of viscoelastic and elastoviscoplastic wake flows at moderate inertia

S. Parvar, A. Corrochano, S. Le Clainche, O. Tammisola

Session 4: 4:05 pm - 5:20 pm

Particle-Laden Flows with Complex Fluids

Célio B. P. Fernandes, Salah A. Faroughi

Modelling and numerical simulation of dilute ferrofluid emulsions

Paolo Capobianchi, Marcello Lappa, Fernando T. Pinho, Mónica S. N. Oliveira

Structure evolution of magnetorheological fluids under balanced triaxial fields and simple shear flow

Jose R. Morillas, Juan de Vicente, Jeffrey F. Morris

Wednesday, 31st May

Session 5: 9:00 am - 10:40 am

The Cytosol viscosity of Red Blood Cells

Christian Wagner

On the absence of collective motion in a bulk suspension of spontaneously rotating dielectric particles

Debasish Das, David Saintillan

Microbial rheotaxis in complex fluids: Shear-thinning effects

Bryan O. Torres Maldonado, Albane Thery, Quentin Brosseau, Paulo E. Arratia

A Swirling Robotic Swimmer Propelled only by Fluid Normal Stresses

Jeremy Binagia, Laurel Kroo, Noah Eckman, Manu Prakash, Neo Boon Siong, Eric S.G. Shaqfeh

Session 6: 11:05 am - 12:45 pm

Data-driven constitutive modeling in fluidic four-roll mill flows via small-angle X-ray scattering

Charles D. Young, Patrick T. Corona, Anukta Datta, Matthew E. Helgeson, and Michael D. Graham

Large Particle-based reverse perturbation algorithms for complex fluids in pure shear and kinematically-mixed extensional-dominated flows

Luke R. Debono, Helen J. Wilson, Luke K. Davis

Extensional Rheometry using Numerically-optimized Stagnation Point Microfluidic Devices

S. J. Haward, F. Pimenta, S. Varchanis, D. W. Carlson, K. Toda-Peters, G. H. McKinley, M. A. Alves, A. Q. Shen

Transport dynamics of spherical microparticles and fibers in inertio-elastic vortex flows

Noa Burshtein, Arash Alizad Banaei, Marine Aulnette, Simon J. Haward, Amy Q. Shen, Anke Lindner

Session 7: 2:00 pm - 4:05 pm

Special session in celebration of Martien Hulsen's work

Square roots' for the modeling and simulation of complex fluids and solids

Markus Hütter, Martien A. Hulsen, Michal Pavelka, Patrick D. Anderson

Tensile tests of poroelastic and poroviscoelastic materials

Antonis Marousis, Pantelis Moschopoulos, Yannis Dimakopoulos, John Tsamopoulos

Modeling and optimization of extrudate swell

Michelle M. A. Spanjaards, Martien A. Hulsen, Patrick D. Anderson

Numerical simulations on the settling dynamics of ellipsoidal particles in non-Newtonian fluids

Gaetano D'Avino

Session 8: 4:05 pm - 5:20 pm

Coffee and Panel Discussion

Thursday, 1^{st} June

Session 9: 9:00 am - 10:40 am

Purely-elastic turbulence in viscoelastic pressure-driven channel flow
Martin Lellep, Moritz Linkmann, and Alexander Morozov

Elastic turbulence pathways of semi-dilute giant micelles in Taylor-Couette flows: the crucial insight into curvature ratio
Xiaoxiao Yang, Darius Marin, Charlotte Py, Sandra Lerouge Anke Lindner

On the near wall structure of the turbulent flow of non-Newtonian fluids: Friction factor and velocity profile
H. R. Anbarlooei, F. Ramos, D. O. A. Cruz

Similarity theory for turbulent planar wakes of viscoelastic fluids
M. C. Guimarães, F. T Pinho, C. B. da Silva

Session 10: 11:05 am - 12:45 pm

Dimensionless numbers in viscoelastic flows
Rafael A. Figueiredo, Cassio M. Oishi, Roney L. Thompson

Viscoelastic Thermally-Driven Flows in Normal and Microgravity Conditions: Laminar and turbulent states
Marcello Lappa, Alessio Boaro, Hermes Ferialdi

Fully Lagrangian Heterogeneous Multiscale Modelling of Non-Newtonian fluids
Nicolas Moreno, Marco Ellero

Recent advances in polymer viscoelasticity from general rigid bead-rod theory
Jeffrey Giacomin, Mona Kanso

Predicting the efficacy of foams in sclerothapy

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Abstract: In varicose vein sclerotherapy, a liquid foam containing sclerosant is injected into the vein to displace blood and to trigger vein collapse. The choice of parameters such as liquid fraction and bubble size are critical in ensuring that the blood is displaced and that the foam then disperses quickly.

Foams exhibit a yield stress at high strain, which depends upon liquid fraction and bubble size. By modelling them as Bingham fluids we can formulate predictions of optimal parameter values. FEM calculations allow more realistic vein geometries to be investigated.

To extend this approach we would like to have bubble-scale information. For example, does the discrete nature of the bubbles in a foam suppress or enhance dead zones? A kinetic model, currently two-dimensional, allows us to predict bubble motion, bubble shape, and local stresses.

Modeling of multiphase displacement flow of foamed fluids in annular geometries

Rafael P. M. Moreira, Mônica F. Naccache

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Abstract: Multiphase displacement in annular geometries is present in many industrial applications involving the substitution of fluids, such as oil and gas well cementing operations, which plays a relevant role in well integrity. For some applications, combining a low-density high compressive strength cement is required, and foamed cement is often used in these scenarios. Foamed cementing involves the generation of a cement slurry with stable suspensions of nitrogen bubbles leading to pressure and temperature dependent densities and non-Newtonian rheology. To properly model the displacement complexity involving foamed fluids, which comprise non-Newtonian behavior and high-compressibility, a 3-dimensional computational fluid dynamics (CFD) model was developed from the open-source OpenFOAM toolbox. The conservation and constitutive equations are solved in an annular geometry, taking the effect of pressure in fluid density and rheology. The volume-of-fluid (VoF) method was used to capture the interface between fluids with low interfacial tension. A validation of the implemented models was performed using exact solutions for axisymmetric single-phase flow with incompressible and compressible fluids, and Newtonian and non-Newtonian constitutive models. Further, the multiphase simulations show the removal efficiency of the drilling fluid by the foamed cement slurry in selected scenarios and different correlations for the foamed cement rheological behavior. The model developed may also be suitable for other applications involving displacement flows of foamed and energized fluids.

A Conservative Level-Set Method for Multiphase Viscoelastic Flows

W. Doherty, T. N. Phillips, Z. Xie

Cardiff University. UK

Presenting author: Tim Phillips, PhillipsTN@cf.ac.uk

Abstract: The development of stable numerical schemes for viscoelastic multiphase flows has implications for many areas of engineering applications. We will describe the implementation of a conservative level-set method to define implicitly the interface between fluid phases, fully integrated into the mathematical framework of viscoelastic flow. The log-conformation formulation of the constitutive equation is used and the governing equations are discretized using the finite element method. The numerical scheme is validated with reference to several benchmark problems. The motion of a gas bubble rising in a viscoelastic fluid is studied in detail. The influence of polymer concentration, surface tension, fluid elasticity and shear-thinning behaviour, on flow features such as the development of filaments and cusps and the generation of negative wakes is explored.

Enhancing the applicability of the elliptic grid methods for flow with moving boundaries

Pantelis Moschopoulos [1], Alexandros Spyridakis [1], Stylianos Varchanis [2], Yannis Dimakopoulos [1], John Tsamopoulos [1]

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Abstract: Resolving the local flow dynamics near moving interfaces is a challenging task. The most accurate methods to do so are those developed under the boundary-fitted framework. Here, we investigate a set of quasi-elliptic equations derived under the framework of variational principles [1-4] to control the motion of the mesh nodes. However, the scheme requires mapping of the physical domain to a simpler computational one, where the interface coincides with a mesh boundary, which can only be a straight line in 2D or a planar surface in 3D. In this work, we aim to lift this limitation by generalizing the equidistribution boundary condition that enables us to use curved computational domains and control the distortion of the mesh elements simultaneously. Using our new method, we capture accurately the knife edge shape of a bubble rising in a viscoelastic material, where the mesh boundary follows readily the anisotropic deformation of the surface. Moreover, we simulate the stretching of a Newtonian bridge, with a fivefold increase in its height without remeshing. These results show the great flexibility and accuracy that the proposed method offers in simulating flows with complex moving boundaries.

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[1] J.U. Brackbill, J.S. Saltzman, J. Comput. Phys. 46 (1982)
[2] K.N. Christodoulou, L.E. Scriven, J. Comput. Phys. 99 (1992)
[3] Y. Dimakopoulos, J. Tsamopoulos, J. Comput. Phys. 192 (2003)
[4] D. Fraggedakis, J. Papaioannou, Y. Dimakopoulos, J. Tsamopoulos, J. Comput. Phys. 344 (2017)

The rheology of non-Brownian suspensions under inhomogeneous flow

Christopher Ness

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Abstract: The homogeneous rheology of dense non-Brownian suspensions is well-characterised by the mu(J) framework proposed by Boyer et al [1]. The behaviour predicted by this model is not observed under inhomogeneous flow, however, and one finds flowing regions with (i) macroscopic friction coefficient below the yielding criterion; (ii) volume fraction above the jamming criterion.

Recent work in dry granular materials [2] found that the granular temperature can be used to collapse inhomogeneous flow data from various geometries to a single master curve. Since the mu(J) result was itself motivated by dry granular rheology, it is tempting to look for an analogous way to unify inhomogeneous data in suspensions. Here we set up a 'computational thought experiment', a highly simplified simulation that produces inhomogeneous rheology data for dense suspensions, and use its predictions to explore whether the temperature (or the velocity fluctuations more generally) plays a similar role in viscous systems as it does in inertial ones.

Our model simultaneously provides an opportunity to examine the relation between particle migration and normal stresses.

[1] Boyer, F., Guazzelli, É. and Pouliquen, O., 2011. Unifying suspension and granular rheology. Physical Review Letters, 107(18), p.188301.
[2] Kim, S. and Kamrin, K., 2020. Power-law scaling in granular rheology across flow geometries. Physical Review Letters, 125(8), p.088002.

Simulations of concentrated suspensions of rough polydisperse particles using tribological friction models

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Presenting author: Jose A. Ruiz-Lopez, jantonio@ugr.es

Abstract: Concentrated suspensions of particles generally exhibits a shear-thickening behavior in the case of repulsive interactions. Although frictional contacts have been able to explain the discontinuous shear thickening (DST) in simulations [1], the causes of the shear-thickening remain unclear. The interparticle friction coefficient is taken as constant [1] in most simulations and theoretical works. Nevertheless, tribological experiments demonstrate that the friction coefficient can not only be constant (boundary regime) but also decrease (mixed regime) or even increase (full-film lubrication regime), depending on the normal force and the relative velocity between the particles and the interstitial liquid between them [2]. Interestingly, the transition between the boundary regime and the full-lubrication regime is governed by the particle average roughness [2].

Particle-level simulations of suspensions of hard spheres were carried out using short-range lubrication and roughness-dependent frictional forces describing the full Stribeck curve [3]. Suspensions with different particle's roughness were simulated to show that the particle roughness is a key factor in the shear-thickening behavior; for sufficiently rough particles, the suspension exhibits a remarkable shear-thickening, while for sufficiently smooth particles, the DST disappears [3]. Simulations using a tribological variable-friction coefficients can be used to explain experimental results with particles with different roughness [4] and also with different solvent viscosities [5].

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[3] J. A. Ruiz-Lopez, et al., J. Rheol. 67, 541-558 (2023).
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[5] Xu, et al., J. Rheol. 64, 379-394 (2020)

Scaling relations between viscosity and diffusivity in shear-thickening suspensions

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Abstract: Dense suspensions are a prototype of fluid that can dynamically enhance its viscosity to resist strong external forcing. Recent work established that the key to a large viscosity increase, often over an order of magnitude, is the ability to switch from unconstrained lubricated particle interactions at low stress to a network of constrained frictional contacts at higher stress. Here, we use numerical simulations to study the flow behavior and shear-induced diffusion of frictional non-Brownian spheres in two dimensions under simple shear flow. We show that both the viscosity and diffusivity of the particles increase at characteristic shear stress associated with lubrication to frictional transition. We propose a one-to-one relation between viscosity and diffusivity using the length scale related to the size of collective motions (rigid clusters) of the particles. We demonstrate that viscosity and diffusivity are controlled by rigid cluster size in two distinct flow regimes, i.e., in the frictionless and frictional states. Finally, we show that the one-to-one relation is described as a crossover from power law 1 (frictionless case) to 1/3 power law (frictional case). We also confirm the proposed power laws are insensitive to friction and system size.

Particle redistribution in a horizontal Couette

Mahdi Davoodi, Andrew Clarke

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Abstract: Drilling of any borehole (artisan, oil or gas, engineered geothermal etc.) requires a drilling fluid. Today, such fluids are highly engineered to maintain well defined rheological properties. Although the fluids are required to support many functions, their primary function is to carry drilled cuttings from the drill bit, along the borehole, and to surface. Whereas for vertical wells this is rather straightforward, most boreholes today have highly deviated or long horizontal sections for which cuttings tend to accumulate on the lower side of the hole and therefore for which transport of cuttings over long distances is problematic. Hence, understanding the interaction of process conditions and fluid properties on cuttings transport is of paramount importance for the successful drilling of a desired borehole.

In this work, we investigate the flow conditions encountered during hole-cleaning processes. For a horizontal well the cuttings transport occurs between the drill-pipe and the borehole, i.e. in a horizontal annular cavity. Typically the drill-pipe rotates and indeed such rotation is routinely used to enhance transport with the guidance of a set of "rules of thumb". We therefore study here particle transport, from a gravitationally formed bed, in a horizontal Couette geometry as a function of inner rotation rate. We have built a detailed 3D, time-dependent, numerical model verified with a range of experimental observations.

In the numerical part of the study we have adapted a Non-Newtonioan constitutive model, originally formulated for simple-shear flow conditions, that describes the stress tensor for a mixture of particles in a Newtonian liquid, into a two-phase finite-volume solver. Here, the mathematical platform describing the interaction of two-phases is obtained using the conservation of mass and momentum in each phase from an Eulerian-Eulerian perspective. The governing equations are coded in a solver developed in-house using OpenFOAM. To extend our investigation and to benchmark the numerical results, a series of detailed experiments have been carried out, initially with Newtonian background fluids (although the composite is non-Newtonian). A purely wall-driven flow condition (i.e., no axial flow), has been used to carry out both the experiments and numerical simulations. Above a critical rotation rate, the well-known Taylor vortex and succession of more complex instabilities replaces the simple azimuthal flow. Using numerical simulations with supporting experimental data, we show that as rotation speed exceeds a further critical

value, particles are lifted from the bed and decorate the Taylor vortices. The fluid secondary motion is shown to be a key element for the solid-bed redistribution and resuspension.

The results obtained from the experiments show excellent agreement with numerical simulations carried out with our numerical solver. The strong agreement suggests the mathematical platform can be successfully used to simulate the interaction of suspended particles with a fluid flow even in complex flow conditions.

Complex viscoplastic flows in superhydrophobic channels: A modeling framework

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Abstract: We investigate the transport of viscoplastic fluids through channels with grooved superhydrophobic walls using a comprehensive modeling approach and numerical simulations. Our goal is to understand the interactions between the fluid and the superhydrophobic surface and identify factors that influence flow behavior. Groove orientation, defined by angle theta, can be longitudinal ($\theta = 0°$), transverse ($\theta = 90°$), or oblique ($0° < \theta < 90°$) with respect to the main flow stream. We assume that the interface between the viscoplastic fluid and trapped air in the Cassie state is flat and we model it using the Navier slip law and Bingham model for viscoplastic rheology. A range of channel thicknesses, characterized by the ratio of groove period to half channel height (L/H), and flow parameters including Bingham number (B), slip number (b), groove periodicity length (L/H), slip area fraction (φ), and groove orientation angle (θ) are considered. Perturbation theory is utilized to derive semi-analytical and closed-form solutions for velocity fields in thick channels, while numerical simulations are employed for both thick and thin channels using the Papanastasiou regularization method. These solutions are developed for all groove orientations, with the oblique case being unique due to the nonlinear effects of viscoplastic rheology, a feature absent in Presenting Newtonian flows. We obtain closed-form relations for the flow mobility tensor and effective slip length, highlighting the strong nonlinear effect of viscoplastic rheology. Linear stability analysis of the homogeneous slip condition for a particular flow configuration ($\varphi = 1$) reveals stabilizing/destabilizing effects of the streamwise/spanwise slip condition on the Poiseuille-Bingham flow.

Synergy between elasticity and plasticity of the fluid in complex internal flows

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Abstract: Elastoviscoplastic fluid internal flows are intrinsic to many industries such as filtration, construction and oil recovery. A computational and experimental investigation of the internal flow of elastoviscoplastic fluids is presented in two complimentary studies. Our primary motivation is to gain insight into the formation of stagnant plug zones in apertures. Although these types of flows are more or less well studied in the context of viscoplastic fluids, the synergy of elasticity and plasticity of the practical yield-stress fluids can have great effects on the flow field which is evident both in the computational and experimental studies. We experimentally study the flow of a Carbopol gel over non-smooth topologies by Optical Coherence Tomography (OCT) and confocal microscopy and compare the observations with numerical simulations using adaptive finite element method based upon the augmented Lagrangian scheme. We propose scalings for quantifying the effect of elasticity and plasticity of the fluid which collapse the data onto master curves irrespective of the shape of the geometries.

Thixo-viscoelastoplastic constitutive modelling using an elastic energy-dissipation measure and its validation in complex flow

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Abstract: In this work, a measure for the energy released by a viscoelastic material in motion is used to model the rheological response of thixo-viscoelastoplastic materials with time-dependent internal structure in the rationale of the Bautista-Manero models. The viscoelastic dissipation function entering this new model-variant is positive definite by construction, and, hence, thermodynamically consistent, particularly obtained via application of the GENERIC framework. The modelling is carried out at both levels of deformation, (i) under ideal simple flows, i.e. shear (steady and oscillatory) and extensional flow, to expose the rheological response the this rheological equation-of-state offers; and (ii) in complex flow, under sphere settling and flow through a circular contraction-expansion. Numerical solutions are obtained with our in-house finite volume/element algorithm and expose the influence of the thixotropic and viscoelastic features of this model. This is evidenced via flow-structure and yield-front representations for semi-diluted and highly-concentrated solutions. Under a viscoelastic regime, vortex-structures reflect a complex interplay between the pure-extensional flow in the centreline and the pure-shear flow deformation along walls and in recirculation-zones. Concerning a plastic regime, enhancement of viscoelasticity and thixotropy, causes yield-front fore-aft asymmetries.

Dynamical analysis of viscoelastic and elastoviscoplastic wake flows at moderate inertia

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Abstract: In this numerical and theoretical work, we study Newtonian, viscoelastic and elastoviscoplastic fluids flow past a circular cylinder at a moderate Reynolds number Re=100 by two-dimensional direct numerical simulations and high-order dynamic mode decomposition (HODMD). The coherent structures in these flows are identified by means of HODMD, applied to a set of velocity or stress snapshots, to reveal the role of yield-stress, elasticity, shear-thinning, and shear-thickening on the wake, and the interplay between vortex shedding and non-Newtonian effects. We find that in the shear-thinning elastoviscoplastic flow, when yield stress increases, the drag coefficient and root mean square of the lift coefficient both decrease, while the length of the recirculation bubble LRB increases. These changes indicate that the wake oscillation amplitude decreases with an increasing yield stress. On the contrary, for uniform viscosity fluids and shear-thickening fluids, the drag coefficient C_D increases at a large Bingham number, and the wake becomes chaotic. The comparison of viscoelastic fluid and EVP fluid reveals that the polymer stresses decay considerably less downstream of the cylinder in the EVP case, indicating that significant stresses persist at large distances. We observe that shear-thinning competes with elastic and yield stresses and counteracts their effect, while shear-thickening enhances elastic and yield stress effects, so that the flow pattern can change from periodic to a chaotic flow.

For uniform viscosity and shear-thickening fluids, the flow pattern turns to chaotic when the yield stress increases, and the structure of the low- and high-frequency HODMD modes characterise this transition and suggests a route to chaos. In this work, we present HODMD as a viable tool to describe also non-Newtonian flows with complex rheology in unstable, chaotic and turbulent flow regimes.

Particle-Laden Flows with Complex Fluids

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Abstract: Fluid-particle transport systems present a significant practical relevance, in several engineering applications, such as oil sands mining and polymer processing. In several cases it is essential to consider that the fluid, in which the particles are dispersed, has underlying viscoelastic characteristics, or the particles are susceptive to be permeable to a magnetic field. For this aim, a novel numerical algorithm was implemented on an open-source finite-volume viscoelastic fluid flow solver coupled with an immersed boundary method, which can also take into account the rigid body motion of magnetic spherical particles surrounded by an external applied magnetic field. The accuracy of the algorithm was evaluated by studying several benchmark flows, namely: (i) the sedimentation of a sphere in a bounded domain; (ii) rotation of a sphere in simple shear flow; (iii) the cross-stream migration of a neutrally buoyant sphere in a steady Poiseuille flow; (iv) sedimentation of two spheres reproducing the drafting, kissing, and tumbling (DKT) phenomenon with and without the presence of an external magnetic field; and (v) the movement of random arrays of magnetic spheres located in 2D and 3D domains.

Modelling and numerical simulation of dilute ferrofluid emulsions

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Presenting author: Paolo Capobianchi, paolo.capobianchi@strath.ac.uk

Abstract: The rheology of a dilute emulsion made of ferrofluid droplets dispersed in a non-magnetisable immiscible liquid has been modelled through a bulk stress model and simulated numerically using a Volume of Fluid approach considering uniform magnetic fields and assuming that both phases obey the Newtonian constitutive law. The results reveal that, for magnetic fields of relatively small intensity, the rheological properties of the emulsion are significantly altered with respect to those observed in the absence of magnetic effects. In particular, an increase in the effective viscosity of the emulsion occurs in conjunction with a reversal of the sign of the two normal stress differences. Comparisons between the results predicted with our rheological model and the numerical experiments provide evidence about the reliability of the model and its ability to predict the rheology of the ferrofluid suspension subjected to uniform magnetic fields.

Structure evolution of magnetorheological fluids under balanced triaxial fields and simple shear flow

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Abstract: Magnetorheological (MR) fluids are suspensions of magnetisable microparticles in a Newtonian liquid. When they are exposed to a uniaxial DC magnetic field, the particles magnetise and interact with each other through forces that, in a first approximation, can be regarded as dipolar ones. In this scenario, particles self-arrange in column-like structures that follow the magnetic field and provide the MR fluid with a resistance to flow. Depending on the particle concentration and field intensity, that behaviour is translated into a viscosity increase or even a yield stress.

The MR fluid rheological response under uniaxial DC fields has been studied for a long time, both experimental and numerically, and it is now quite well-understood. In this work we study the MR fluid structure and rheological response under balanced triaxial magnetic fields. Those are fields that change their intensity and direction periodically in time. The characteristic period is so short that suspended particles eventually feel time-averaged forces. The key feature of those forces is their multi-body nature. To compute them properly a previous step is needed where the total magnetic field, the applied one plus the perturbations coming from all suspended particles, on each particle is determined [1].

Through particle-level simulations, we compute the local field and show how under the action of the (triaxial field) time-averaged forces and simple shear the particles arrange in sheets lying with orientation close to the flow-vorticity plane. Because of the fact those sheets cannot bear a shear stress, as the particle population forming sheets increases the MR fluid experiences a transient behaviour where the viscosity continuously decays with time in striking contrast to the common MR fluid response under DC fields.

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The Cytosol viscosity of Red Blood Cells

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Abstract: Red blood cells (RBCs) are known for their deformability, which allows them to squeeze through the smallest of capillaries. In larger vessels, their deformability and their adhesive interactions lead to the well-known shear-thinning, but also to a vessel size dependent viscosity due to the cell-free layer and to margination of white cells. A quantitative comparison of simulations of RBC flow in capillaries with experimental results requires a set of cell membrane parameters as well as the viscosity ratio of the intercellular liquid (cytosol) and the outer liquid as blood plasma. The cytosol consists mainly of solved hemoglobin and some other proteins. We present a procedure to extract that cytosol from the RBCs to perform macroscopic rheology. By centrifugation in density gradients (Percoll), we were able to determine the distribution function (pdf) of individual cell mass densities in RBC samples. Thus, using the above viscosity-density relation and the convolution with the pdf, we can determine the mean cytosol/plasma viscosity ratio, and even the distribution of this ratio for RBCs. The viscosity ratio was determined to be 15 with a width of +/-5. This is significantly higher than the ratio of 5 previously used in many simulations, but in agreement with a recent comparison of numerical results and experimental data of RBC dynamics in pulsating channel flow.

On the absence of collective motion in a bulk suspension of spontaneously rotating dielectric particles

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Abstract: A suspension of dielectric particles rotating spontaneously when subjected to a DC electric field in two dimensions next to a no-slip electrode has proven to be an ideal model for active matter [Bricard *et al., Nature*, 2013, **503**, 95–98]. In this system, an electrohydrodynamic (EHD) instability called Quincke rotation was exploited to create self-propelling particles which aligned with each other due to EHD interactions, giving rise to collective motion on large length scales. It is natural to question whether a suspension of such particles in three dimensions will also display collective motion and spontaneously flow like bacterial suspensions do. Using molecular dynamics type simulations, we show that dielectrophoretic forces responsible for chaining in the direction of the applied electric field in conventional electrorheological fluids prevent collective motion in suspensions undergoing spontaneous particle rotations. Our simulations discover that the fundamental microstructural unit of a suspension under Quincke rotation is a pair of counter-rotating spheres aligned in the direction of the electric field. We perform a linear stability analysis that explains this observation.

Microbial rheotaxis in complex fluids: Shear-thinning effects

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Abstract: The positive rheotaxis of microorganisms encompasses the spontaneous orientation of individual swimmers against a unidirectional flow. Much progress has been made in understanding the physical mechanisms governing this phenomenon in Newtonian liquids; much less is known for the case when microorganisms encounter non-Newtonian fluid flows. Here, we show how shear-thinning viscosity behavior can significantly enhance the rheotactic behavior of the bacterium E. coli near walls. Experiments show that shear-thinning effects suppresses E. coli curved trajectories leading to alignment against the imposed flow. A simple model based on a rotating cylinder near wall seems to capture the experimental observations relatively well.

A Swirling Robotic Swimmer Propelled only by Fluid Normal Stresses

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Abstract: Recently, there has been interest in developing artificial micro-swimmers that leverage the complex rheology of their surrounding fluid. Such synthetic micro-swimmers could be used for a variety of applications, including as portable, self-propelling rheological probes. To this end, we've studied a simple force- and torque-free swimmer consisting of two counter-rotating bodies of revolution. This swimmer is realized experimentally as a battery-powered robot, where an optical signal is used to control the relative rotation rate of the two halves of its body. Using a combination of theory, numerical simulations, and experiments, we demonstrate that such a swimmer displays no net translation in a Newtonian fluid at low Reynolds numbers but does exhibit net translation when placed in a viscoelastic fluid.

In the case of two counter-rotating spheres, we develop an asymptotic theory showing that at zero Reynolds number and low Deborah number, the swimming speed is approximately linear in Deborah number.

To better understand the moderate De regime, we also performed numerical simulations of this swimmer using a multi-mode Giesekus constitutive model, which captures the effects of shear-thinning and multiple relaxation timescales in the fluid. With no fitting parameters, we show good agreement between experiments and numerical predictions in swimming speed across a range of De.

Furthermore, by exploring a range of relative sizes and shapes (cones, cylinders, etc) for the two halves of the swimmer, we can determine the geometry that maximizes the swimmer's speed. We conclude by discussing how observation of both the forward propulsion speed and the relative rotation of the two halves of the swimmer can be used to infer rheological properties of the surrounding fluid. Finally, we demonstrate how oscillations of the swimmer "tail" can be used to determine the spectrum of relaxation times in a fluid via a measurement akin to linear viscoelasticity.

Data-driven constitutive modeling in fluidic four-roll mill flows via small-angle X-ray scattering

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Abstract: Two challenges in learning rheological models from data are the availability of training data sets and the measurement of sample deformations under mixed rotational and extensional flows commonly encountered in processing applications. We address these challenges using data from scanning small-angle X-ray scattering (sSAXS) measurements in a fluidic four-roll mill (FFoRM). The FFoRM-sSAXS approach provides a large data set of nanostructural measurements along diverse 2D Lagrangian deformation trajectories. We propose a machine learning framework in which FFoRM-sSAXS data is used to train a model which can predict the nanostructural evolution of the fluid for an arbitrary deformation (velocity gradient tensor) input. We first use autoencoders to learn a reduced order model from scattering data. We then learn the time evolution in the reduced state using a neural network approximation to the governing differential equation. Finally, we learn a transformation from the state data embedded in the scattering intensity to the stress exerted on the fluid. We incorporate frame indifference by performing data-driven operations in a co-rotating frame determined completely by the deformation input. The framework is tested on a rigid rod suspension and compared to theoretical constitutive models and bulk rheological data.

Particle-based reverse perturbation algorithms for complex fluids in pure shear and kinematically-mixed extensional-dominated flows

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Abstract: In this talk, I begin with an overview of traditional methods for extracting the viscosity from non-equilibrium molecular dynamics simulations. Following this, we discuss the concept of reverse perturbations and the utility of these algorithms in systems where momentum exchange between particles is not easily defined. On this foundation, the Müller-Plathe reverse perturbation algorithm [1] will be introduced and some key numerical and physical properties will be discussed.

To reach beyond simple shear, I introduce a novel reverse perturbation algorithm for simulating kinematically-mixed extensional flow-dominated systems. This method which is still in the development stage is akin to the four-roll mill extensional rheometer. Assuming the successful implementation of the algorithm, I finish this talk by suggesting a data processing method for extracting extensional and shear viscosity.

[1] Müller-Plathe, F. (1999). Reversing the perturbation in nonequilibrium molecular dynamics: An easy way to calculate the shear viscosity of fluids. Physical Review E 59 (5).

Extensional Rheometry using Numerically-optimized Stagnation Point Microfluidic Devices

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Abstract: Numerically-optimized stagnation point microfluidic devices are used to compare the extensional rheological properties of dilute polymer solutions under the three fundamental modes of extension. The optimized shape cross-slot extensional rheometer, OSCER [1] is used to apply planar elongation, while a new device (the optimized uniaxial and biaxial extensional rheometer, OUBER [2]) is used to apply both uniaxial and equibiaxial elongational flows. Polymer solutions are formulated from dilute concentrations of a 5 MDa nonionic polyacrylamide in an aqueous glycerol solvent. In each of the three microfluidic extensional flows, the extension rate $\dot{\varepsilon}$ is quantified using microparticle image velocimetry and the principal stress difference as a function of $\dot{\varepsilon}$ is estimated from pressure drop measurements. For the most dilute polymer sample (which is considered "ultradilute"), the extensional viscosity is very well described by the FENE P model, where at high $\dot{\varepsilon}$ the limiting biaxial extensional viscosity is 50% of the uniaxial and planar extensional viscosities. At higher polymer concentrations, the experimental measurements deviate from the model predictions, which is attributed to the onset of intermolecular interactions as polymers unravel in the extensional flows. Of practical significance (and fundamental interest), elastic instability occurs at a significantly lower $\dot{\varepsilon}$ in uniaxial extensional flow than in either biaxial or planar extensional flow, limiting its utility for extensional viscosity measurement.

[1] S. J. Haward, et al., Phys. Rev. Lett, 109, 128301 (2012).
[2] S. J. Haward, et al., J. Rheol., submitted (2023), http://arxiv.org/abs/2302.10401.

Transport dynamics of spherical microparticles and fibers in inertio-elastic vortex flows

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Abstract: Spherical particles and fibers are common in biological and environmental flows and are used in numerous industrial and pharmaceutical applications. Their motion and flow dynamics are strongly affected by their interactions with the flow structure. While the interaction between particles and flows has been intensely studied in small Reynolds number flows as well as in fully developed turbulence, the transport mechanisms of these particles in intermediate flow regimes remains to be explored. Here we focus on the response of spherical particles and fibers to a single vortex flow field. For this purpose, we use a microfluidic cross-slot geometry, to generate a well characterized, stationary, three-dimensional streamwise vortex at moderate Reynolds number. The controlled vortical flow field allows studying the transport of neutrally buoyant spherical micro-particles and fibers suspended in Newtonian and weakly elastic fluids. Our experimental results, supported with numerical simulations, show that as the diameter of the spherical particles are increased, they are progressively expelled from the vortex core. This trend is further enhanced when the fluid's elasticity is slightly increased. Initial observations also indicate a complex interaction between fibers and a vortical flow field, in which the fibers can rotate, and either follow or diverge from the streamlines depending on their size and initial orientation. This work provides a fundamental contribution to the study of particle–flow interactions and for the improvement of particle sorting and transport techniques with possible environmental, industrial and pharmaceutical applications.

Square roots' for the modeling and simulation of complex fluids and solids

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Abstract: The conformation tensor is often used for the description of polymer solutions and melts. However, we argue that it may be beneficial to consider instead its multiplicative decomposition, i.e., to use its "square root" [1], with the following advantages: On the one hand, the numerical stability of FEM calculations is enhanced [2] particularly with respect to the High Weissenberg Number Problem, and on the other hand, it is significantly more convenient for incorporating thermal fluctuations at small scales [1,3]. While the square root is not unique, it is shown how gauge conditions can be employed to achieve uniqueness [4], which is essential for testing the stability and convergence of square-root based models. Furthermore, a comparison will be made between the square root of the conformation tensor on the one hand, and the elastic part of the deformation gradient commonly used in the modeling of complex solids on the other hand. In particular, our recent efforts suggest that, also with respect to multiscale modeling, an Eulerian theory of solids should employ not the (elastic part of the) deformation gradient as fundamental variable, but rather its inverse [5]. Does this have implications for the modeling of complex fluids?

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[2] M.A. Carrozza, M.A. Hulsen, M. Hütter, P.D. Anderson, J. Non-Newtonian Fluid Mech. 270:23-35 (2019)
[3] M. Hütter, M.A. Carrozza, M.A. Hulsen, P.D. Anderson, Eur. Phys. J. E 43:24 (2020)
[4] M. Hütter, H.C. Öttinger, J. Non-Newtonian Fluid Mech. 271:104145 (2019)
[5] M. Hütter, M. Pavelka, Continuum Mech. Thermodyn., submitted (2023)

Tensile tests of poroelastic and poroviscoelastic materials

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Abstract: Soft porous materials exhibit elastic or viscoelastic mechanical properties because of their deformable solid matrix, which interacts with the entrapped liquid (poromechanical coupling). Also, they expand when a liquid is injected into their porous and shrink when they are compressed, driving the liquid out. The present study is focused on the numerical simulation of the elongation and compression of soft porous materials. The numerical schemes proposed by Varchanis et al. (2019) and (2020) are appropriately modified for simulating the above-mentioned type of flows in the context of large-deformation poroelasticity using a Lagrangian reference frame, typically fixed to the solid matrix. The effect of the permeability of the porous medium, the viscoelastic properties of the solid matrix, and the viscous properties of the fluid are parametrically studied.

This work is part of the Research Project "Multiscale modeling for the autoregulation of Microvessels, CARE" which was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the "1st Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment" (Project No. 81105).

[1] Varchanis, S., Syrakos, A., Dimakopoulos, Y., and Tsamopoulos, J. (2019). A new finite element formulation for viscoelastic flows: Circumventing simultaneously the LBB condition and the high-Weissenberg number problem. Journal of Non-Newtonian Fluid Mechanics, 267, 78–97. doi:10.1016/j.jnnfm.2019.04.003

[2] Varchanis, S., Syrakos, A., Dimakopoulos, Y., and Tsamopoulos, J. (2020). PEGAFEM-V: A New Petrov-Galerkin Finite Element Method For Free Surface Viscoelastic Flows. Journal of Non-Newtonian Fluid Mechanics, 104365. doi:10.1016/j.jnnfm.2020.104365

Modeling and optimization of extrudate swell

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Abstract: Extrusion is a widely used process to create products with a fixed cross-sectional shape. Many applications require complex shaped cross-sections, where the dies contain sharp corners. Common requirement on the extrudate is dimensional precision. However, the shape and dimensions of the extrudate are highly influenced by a phenomenon called extrudate swell. The swelling process involves complex dynamics influenced by many parameters, such as viscoelasticity and temperature. Therefore, the optimized shape of a die, to obtain an extrudate with desired dimensions and shape, is now often obtained through trial-and-error.

We developed a transient 3D finite element model, to predict extrudate swelling for extrudates containing sharp edges. This model describes the corner lines of the domain separately to obtain the positions of these lines in the two swell directions. A 2D height function is used to describe the free surfaces of the extrudate, using the positions obtained from solving the material lines to expand the domain of the height function [1].

This method is combined with a real-time active control scheme, to numerically solve the inverse problem of three-dimensional die design for extrudate swell. A feedback connection is established between the finite element method and the control scheme [2]. In this talk we show that this is a promising approach to design dies for viscoelastic extrusion flows. Furthermore, we will highlight the applicability of the developed method to model various extrusion techniques for complex materials. Preliminary results of a 2D coextrusion model for different fluid layers separated by sharp interfaces will be shown.

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[2] M.M.A. Spanjaards, M.A. Hulsen, P.D. Anderson. Journal of Non-Newtonian Fluid Mechanics, 293:104552, 2021

Numerical simulations on the settling dynamics of ellipsoidal particles in non-Newtonian fluids

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Abstract: Sedimentation of particles immersed in non-Newtonian fluids occurs in a variety of industrial applications. The falling dynamics and the terminal velocity attained by the particle depends on the magnitude of the applied force, the particle shape, and the rheological properties of the suspending fluid. Although the settling of spherical particles in non-Newtonian liquids has been thoroughly investigated, only few studies are available for particles with anisotropic shapes, limited to axisymmetric geometries (e.g., cylinders or spheroids) and mainly focused on the final orientation attained by the particle.

In this work, we carry out extensive 3D finite element simulations to study the dynamics of a rigid particle with triaxial ellipsoidal shape immersed in an unbounded viscoelastic fluid and subjected to a constant force. An Arbitrary Lagrangian-Eulerian formulation is adopted to handle the particle motion. The effect of the Weissenberg number, particle aspect ratios (including oblate and prolate spheroids), and initial orientation on the settling dynamics is addressed. The flow and stress fields around the particle are inspected in order to evaluate the possible formation of a negative wake behind the particle and its relation with shape anisotropy. The steady-state drag correction coefficient as a function of the particle aspect ratios is computed. Preliminary simulation results on the settling dynamics of spheroids in an elastoviscoplastic fluid are also presented.

Purely-elastic turbulence in viscoelastic pressure-driven channel flow

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Abstract: Dilute polymer solutions do not flow like Newtonian fluids. Their flows exhibit instabilities at very low Reynolds numbers that are driven not by inertia, but rather by anisotropic elastic stresses. Further increase of the flow rate results in a chaotic flow, often referred to as purely elastic turbulence (PET). The mechanism of this new type of chaotic motion is poorly understood.

We consider a model shear-thinning viscoelastic fluid driven by an applied pressure gradient through 2D and 3D channels. By starting from a linearly unstable mode recently discovered by Khalid et al. (Khalid et al., Phys. Rev. Lett. 127, 134502 (2021)) at very large flow rates and very low polymer concentrations, we demonstrate the existence of 2D travelling-wave solutions in such flows. We show that this state sub-critically connects to significantly higher values of polymer concentration and lower flow rates (Morozov, Phys. Rev. Lett. 129, 017801 (2022)), rendering travelling-wave solutions experimentally relevant.

Upon embedding the 2D coherent states in a 3D domain, we observe the emergence of a time-dependent, turbulent-like state, that becomes more complex with increasing Weissenberg number. We perform extensive characterisation of the ensuing dynamics and demonstrate its connection to PET.

We acknowledge funding support from the Studienstiftung des deutschen Volkes and Priority Programme SPP 1881 of the DFG Li3694/1. Also, we thank EPSRC for providing computational time on the ARCHER2 UK National Supercomputing Service through the UK Turbulence Consortium (Grant No. EP/R029326/1).

Elastic turbulence pathways of semi-dilute giant micelles in Taylor-Couette flows: the crucial insight into curvature ratio

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Abstract: Elastic turbulence (ET) has been revealed as a spatially smooth and temporally random flow, essentially resulting from the significant coupling of rapid cycles of polymer stretch/relaxation and the fluctuating velocity field. The transition to ET was found to be hysteretic, and strongly subcritical with the occurrence of shear stress jumps above a critical Weissenberg number (Wi). We have observed a very similar phenomenology for shear-banding (SB) giant micellar solutions in Taylor-Couette (TC) flow. Here we extend this study to the investigation of the role of the curvature ratio (Λ) on the onset of ET. We find surprisingly that as a function of curvature ratio the nature of the transition towards purely ET in TC flow of giant micelles may change from subcritical to supercritical even though finite-size effects may also come into play. Two distinct transitional pathways to ET are identified. One is proceeding via a flow relaminarization phenomenon following the 3D SB regime subsequently leading to a sudden subcritical transition to ET accompanied by a shear stress jump and a hysteretic loop at the lowest Λ. Another pathway is featured by a regime of elastic turbulent bursts triggered inside the 3D SB regime and eventually eliminated by ET, the suppression of the shear stress jump and shift of the onset of ET towards smaller Wi when increasing Λ. A universal state diagram can be established in the parameter space of Λ-Wi, independent of the type of micellar systems. Furthermore, the onset of ET is observed to follow a general scaling criterion, which is reminiscent of the renowned elastic instabilities criterion established by Pakdel and McKinley. It would be very useful to compare our results with numerical simulations.

On the near wall structure of the turbulent flow of non-Newtonian fluids: Friction factor and velocity profile

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Abstract: One of the most challenging and yet not well understood phenomena related to the turbulent flow of non-Newtonian fluids is the momentum transfer mechanism at the near wall region. Both the friction factor and the shape of the velocity profile are directly connected to the vortex pattern at the maximum turbulent shear stress region, which is related to the so-called mesolayer. In this work, an attached eddy hypothesis (AEH) is formulated for non-Newtonian fluids to model the momentum transfer at the mesolayer, so that we can extend recent results obtained for Newtonian fluids to non-Newtonian turbulent flows. Some new friction relations for power law fluids and viscoelastic fluids will be presented and a new velocity profile is also shown. For power law fluids, the proposed velocity profile is valid for both the inner and outer regions, reproducing the log law behavior at the inner region and reducing to a power law behavior (u+ = a y+ b) for large values of y+. For viscoelastic fluids, a friction equation is obtained using the Oldroyd model. The new relation describes accurately the maximum drag reduction limit. The results are compared with experimental data and DNS simulations show excellent agreement.

Similarity theory for turbulent planar wakes of viscoelastic fluids

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Abstract: A similarity analysis of the governing equations for the mean conformation tensor (*Cij*) and its trace (*Ckk*) is carried out for turbulent planar wake flows of viscoelastic solutions to develop a theory for their evolution in the far-field, where turbulence is fully-developed. The fluid is described by the FENE-P model and results obtained from Direct Numerical Simulations (DNS) in long domains are used to assess the theory at different Reynolds (Re) and Weissenberg numbers (Wi), viscosity ratios (β) and maximum polymer extensibilities (L). Provided the inlet Wi is high, the far-field is composed of two main regions of viscoelastic effects, the highly elastic region, where polymers are highly stretched, followed by the nearly-coiled low elasticity region.

In the former the total rate of dissipation of turbulent kinetic energy (k) is predominantly by the polymer, hence the solvent dissipation reduction (SDR) attains its maximum, which is independent of the streamwise coordinate x, Re, Wi, β and L. Polymers are initially highly stretched in an anisotropic configuration where mean stretching and mean flow advection produce -*Cxy*, whereas mean relaxation and turbulent stretching reduce it (similarly for the normal components of *Cij*, with exceptions due to symmetry conditions). Then they acquire a nearly-isotropic configuration where mean and turbulent stretching essentially balance for -*Cxy*, whereas the turbulent stretching balances mean relaxation for all normal components.
In the nearly-coiled region, the polymer configuration is nearly-isotropic and subsequently viscoelasticity goes into a final region of decay. In the former, as in the nearly-isotropic sub-region of the highly elastic region, polymer stretching is essentially imposed by the approximately isotropic intermediate and small-scale turbulence. In this region solvent and polymer contribute to the total rate of dissipation of k, with the polymer assuming a dissipative role proportional to its low shear rate viscosity. SDR has its lowest value, linearly proportional to 1-β, but independent of x, Wi and Re.

The analytical theory, confirmed by DNS, provides adequate scaling laws for all components of *Cij* in all sub-regions as a function of inlet and rheological conditions and x.

Dimensionless numbers in viscoelastic flows

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Abstract: The Reynolds number was conceived in a Newtonian, incompressible, isothermal paradigm. Hence, any deviation from this condition, such as a viscosity function, a density function, or properties that depend on temperature, distorts this dimensionless number in a complex manner. In a similar fashion, the Weissenberg number was conceived in a Maxwell/Oldroyd paradigm, where relaxation is constant. When viscoelastic fluids of intermediate complexity (one additional parameter with respect to the Oldroyd-B constitutive equation), such as PTT or Giesekus, are subjected to a flow, Reynolds and Weissenberg numbers are generally interpreted as expressions, instead of being constructed by their physical meaning. This interpretation induces misleading conclusions, where the role of the parameter associated with the nonlinear effect is overestimated. In other words, the Presenting Oldroyd-B case, which serves as a reference for comparison of the results obtained by nonlinear models is not judiciously chosen. In the present work, we construct Reynolds and Weissenberg numbers from their physical meaning and we use viscoelastic flow simulations of the classical 4:1 abrupt contraction to illustrate the points raised above. We show that Coutte correction and recirculation size are less affected by the nonlinear parameter than then the literature suggests. The procedure adopted needs a base flow, in this case, a viscometric flow between parallel plates, in order to capture the characteristic viscosity and characteristic relaxation time, needed to compose Reynolds and Weissenberg numbers.

Viscoelastic Thermally-Driven Flows in Normal and Microgravity Conditions: Laminar and turbulent states

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Abstract: A survey is provided of recent numerical results concerning the dynamics of thermal convection in visco-elastic fluids subjected to thermal stimuli of various kinds (heating from below or from the side) and driving forces. The considered flows encompass canonical realizations of thermo-gravitational and surface-tension driven flows such as those obtained when the considered fluid is heated from below (namely, Rayleigh-Bénard and Marangoni-Bénard convection, respectively), and more exotic variants, such as those induced in microgravity conditions by the application of time-varying accelerations with a zero mean value (thermovibrational convection). The goal is to illustrate recent developments about the behaviour of all these forms of convection in the respective non-linear (finite-amplitude) states for the cases where the so-called concept of overstability is applicable. These problem are tackled through numerical solution of the three-dimensional Navier-Stokes and energy equations, properly cast in the framework of the Oldroyd-B or FENE-CR paradigms. An attempt is made to distillate some common ground by highlighting analogies and differences and interpreting the observed phenomena in the context of existing theories related to spatially localised oscillatory structures in fluid flow (the so-called oscillons), competing multiple solutions (i.e. states which exhibit SIC), strange attractors and elastic vs Kolmogorov turbulence.

Fully Lagrangian Heterogeneous Multiscale Modelling of Non-Newtonian fluids

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Abstract: We propose a full-Lagrangian heterogeneous multiscale method (LHMM) to model non-Newtonian fluids with microscopic effects that affect the flow over large spatial and temporal scales (e.g. polymeric solutions and multiphasic systems). The proposed approach discretizes the fluctuating Navier-Stokes equations using the Smoothed Dissipative Particle Dynamics (SDPD) method. The LHMM uses microscopic information derived on-the-fly to provide the stress tensor of the momentum balance in a macroscale problem. Henceforth, it does not require approximating constitutive relations to obtain the stress. The LHMM allows for a hybrid stabilized scheme where the ideal contribution of the stresses can be computed either from macro, microscale or a weighted average of both. We validate the LHMM for Newtonian and non-Newtonian fluids, using different flow configurations such as reverse Poiseuille flow, flow passing a cylinder array, and flow around a square cavity.
We showed the framework's flexibility to model complex fluids at the microscale using multiphase and polymeric systems. We evidence that the stresses are adequately captured and passed across scales, leading to a richer fluid response at the continuum level. In general, the proposed methodology provides a natural link between variations at a macroscale, while accounting for the memory effects of microscales.

Recent advances in polymer viscoelasticity from general rigid bead-rod theory

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Abstract: One good way to explain the elasticity of a polymeric liquid, is to just consider the orientation distribution of the macromolecules. When exploring how macromolecular architecture affects the elasticity of a polymeric liquid, we find general rigid bead-rod theory to be both versatile and accurate. This theory sculpts macromolecules using beads and rods. Whereas beads represent points of Stokes flow resistances, the rods represent rigid separations. In this way, how the shape of the macromolecule affects its rheological behavior in suspension is determined. Our work shows the recent advances in polymer viscoelasticity using general rigid bead-rod theory, including advances applied on the coronavirus. The coronavirus is always idealized as a spherical capsid with radially protruding spikes. However, histologically, in the tissues of infected patients, capsids in cross section are elliptical, and only sometimes spherical. This capsid ellipticity implies that coronaviruses are oblate or prolate or both. We call this diversity of shapes, pleomorphism. Recently, the rotational diffusivity of the spherical coronavirus in suspension was calculated, from first principles, using general rigid bead-rod theory. We did so by beading the spherical capsid, and then also by replacing each of its bulbous spikes with a single bead. In this paper, we use energy minimization for the spreading of the spikes, charged identically, over the oblate or prolate capsids. We use general rigid bead-rod theory to explore the role of such coronavirus cross-sectional ellipticity on its rotational diffusivity, the transport property around which its cell attachment revolves. We learn that coronavirus ellipticity drastically decreases its rotational diffusivity, be it oblate or prolate.

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