Conference Report

International Workshop on Mesoscale and Multiscale Description of Complex Fluids – IWMMCOF '06

iwmcof 2006

Prato, Italy
July 5 – 8, 2006

The International Workshop on Mesoscale and Multiscale Description of Complex Fluids, was held in beautiful Prato, Italy at the Prato-Monash Center on July 5 - 8, 2006. Ravi Prakash Jagadeeshan (Reader, Monash University, Clayton, Australia) and Eric S.G. Shaqfeh (Professor, Stanford University, Stanford, CA) planned and organized an international conference focusing on the central intellectual themes of modeling complex fluids. The central idea of that conference was that if a broad spectrum of world-reknown scientists were brought to a single location to discuss their modeling problems/issues that general themes would emerge across different modeling efforts, and significant progress could thereby be fostered.

The conference was therefore organized along themes associated with general modeling issues and physical behaviors rather than on any single fluid or groups of fluids. The general modeling issues that formed the titles of the sessions included "Thermodynamics and Coarse-graining issues", "Phase behavior and dynamics", "Linear and nonlinear Rheology" and "Multiscale Modeling". Within each of these general themes a distinguished set of keynote speakers was planned and surrounding each keynote a small set of related invited talks were organized. A single serial set of speaking sessions formed the focus of the workshop, however there were two discussion sections that were also organized. These discussion sessions were led by the keynote speakers and composed of distributed round table meetings. A discussion summary was presented by the keynotes to all participants at the end of the discussion session. Lively and extended discussions marked both the question and answer periods surrounding the invited talks as well as the discussion sessions.

In the area of Thermodynamics and Coarse-graining Issues, E. Sevick, and R.M.L. Evans were the keynote speakers and Sevick led the appropriate discussion session. The discussion focused on the recently developed fluctuation dissipation theorems (the so-called FTs) which have been developed to describe nonequilibrium fluctuating systems. These go by many names including the Jarzynski relations, but all involve theorems on energy trajectories in nonequilibrium systems. Generally, the workshop talks were aimed at elucidating whether these theorems had been established by experiment and whether any useful predictions could be made from them. The issue was put forward that computer simulation might be the key to both proving the validity and usefulness of these theorems since via the computer one can precisely chose the initial conditions of the energy trajectories as well as provide more extensive sampling of the trajectories for statistical analysis.

In the area of Phase Behavior and Dynamics, N. Wilding, M. Cates, and M. Pasquali gave the keynotes. The talks and discussions surrounded issues including colloidal particle/polymer gels, "active" suspensions, particle-laden

Figure 1 (left): Participants at the IWMMCOF '06 in the terrace of the Pallazo Vaj

Figure 2: Burkhard Dünweg (center) asks a question during the IWMMCOF '06. Jay Schieber at right leads the discussion.

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drop emulsions, shear banding, yield stress materials, and carbon nanotubes.

Discussions for gels included the recommendations that a focus on the general properties and the relationship between structure and thermodynamics would point the way to progress. Moreover, in polymer/particle systems computer algorithms play and will continue to play an important role, but relaxation of the system over very long time scales needs to be addressed. Thus a multi-time scale approach should be applied. In terms of physical interactions in particle/polymer gels, the participants felt that we need to move beyond the depletion potential or at least modify this potential to include multi-body interactions.

The discussion surrounding yield stress fluids focused on the finite velocity seen in most experiments at the yield point. Various suggestions were made regarding rheological models for this type of fluid, including the idea that the dynamic friction between complex fluid elements lies below the static friction level.

Finally, carbon nanotubes were found by all workshop members to be extremely interesting materials but their tremendous potential applications are limited by the processing of the liquid phase - the latter of which is very poorly understood. This research area brings together the broad fields of both colloid and polymer science. There was lively debate as to whether carbon nanotube systems would soon play the role of model semi-flexible rod systems or whether the systems are too sensitive to the chemistry of their creation and dispersion in liquids in order to be useful as models.

The keynote speeches in Linear and nonlinear Rheology were delivered by F. Mackintosh, R. Larson A. Sood, and G. McKinley Discussion issues included blood damage in blood pumps, cross-linked semi-flexible biopolymers, rheology in micro/nano fluidics, entangled polymer interfaces, and shear banding and rheo-chaos in micellar systems

Cross linked and non-cross-linked networks of biopolymers were discussed as a common and important complex fluid in biological systems. It was felt that the general aspects of these systems were not yet understood, nor in many cases whether actual cross-linking existed. Failure of the networks was considered as one means of determining the degree and existence of cross-linking and research efforts in that area were encouraged.

The rheology and dynamics of long chain biopolymers in microfluidics was shown to be highly nonlinear because of the presence of nonlinear flow along the chain itself. Glassy configuration states in this context were demonstrated and the verification of this by detailed experiments was encouraged.

Polymer blend systems, both miscible and immiscible, were discussed with the main issues surrounding tube modeling for chains that penetrate the interface. The questions of how the tube changes in terms of its diameter and friction coefficient were considered to be unsolved and determining these as a function of blend composition was considered a topic of future important research.

The lively discussion surrounding shear banding focused on the idea that although shear bands have generally been thought of as a state that results from an instability associated with the decrease of shear stress with increasing strain rate, in fact the bands themselves are almost always unstable. So there appears to be at least the promise of a new way of thinking here. Moreover, materials which show shear bands, such as micellar systems are also prone to rheo-chaos at high shear rates. However, the relation between this chaos and the fluid rheology is not known and again the subject of future important inquiries.

Finally, in the area of Multiscale Modelling, keynotes by M. Kröger and B. Khomami were delivered. The discussion issues and talks were broad ranging but ultimately focused on consistent closure schemes and coarse graining issues. It was generally felt, in a wide range of situations, that closing a complex dynamic set of equations had not been a promising approach and failed to even qualitatively capture the physics involved. Generally, the coupling of stochastic microscale equations with macroscale PDEs was viewed as a much more favorable approach.

It was felt by all participants that this framework for a complex fluids workshop including bringing together participants from a wide range of disciplines who do not normally work together was very successful. More workshops organized in this spirit should be planned in the future.

Eric S.G. Shaqfeh
Ravi Prakash Jagadeeshan