

ESF Exploratory Workshop on

Microfluidic: Experiments and Numerics

SCIENTIFIC REPORT

Castel Gandolfo (near Rome), Italy, 27 - 30 September 2007

Convened by:
Sauro Succi^①, Luca Biferale^② and Federico Toschi^①

^① Consiglio Nazionale Ricerche (CNR)

^② Department of Physics, Universita di Roma II "Tor Vergata"

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EXECUTIVE SUMMARY

The workshop was funded by the ESF and by the ONRG. It was held at “Villa Mondragone” (Monte Porzio, Rome) the conference center of the University of Tor Vergata, from Sept. 27 till Sept. 30, 2007.

The aim of the workshop was to bring into contact scientists from mathematics, theoretical and experimental physics, engineering and industries all working with different perspectives on Microfluidic Flows. The workshop was very successful, as demonstrated by the high standards of the talk and of the informal discussions. Most of the talks were concentrated on investigating meso-scale and nano-scale dynamics affected by micro-scale and nano-scale non-equilibrium effects in fluids.

We have focused on problems spanning a wide range of theoretical and applied issues such as:

- (i) slippage properties of single-phase and two-phase flows at the boundaries of microdevices;
- (ii) mixing properties of passive and active contaminants;
- (iii) viscoelastic effects at the microscales;

First, two long reviews, one on experimental results and the other on basic theoretical challenges have been presented by Tabeling (France) and Eggers (UK) respectively.

For the first issue, we have had experimental, numerical and theoretical talks concerning: the nature of the dynamical wetting transitions (Andreotti, France); phase-field approach to the dynamics of a fluid near a structured wall (Biben, France); Surface effects in fluid dynamics (Boucquet, France); Modeling of dynamic wetting using the lattice Boltzmann method (Care, UK); Molecular dynamics of fluids in patterned nanochannels (Cieplak, Pol); Measurement of Boundary Slip in highly confined flows of Newtonian Liquids (Craig, AUS); Diffuse- and sharp-interface calculations of wetting success and failure (Jacqmin, USA); Modelling Boundary Slip Phenomena in The Lattice Boltzmann Equation (Biferale, Ita); Modelling drops on superhydrophobic surfaces (Yeomans).

Concerning the second issue we have had presentations on: Experimental studies of slippage of water past super hydrophobic surfaces (Cottin-Bizonne, France); Light driven devices and sensors for microfluidics (Di Leonardo, IT); Lattice Boltzmann simulations of phase separation in thermal nonideal fluids (Gonnella, IT); Roughness induced apparent slip in microchannel flows (Harting, Germ); Capillary Rise in Nanopores: Molecular Dynamics Evidence for the Lucas-Washburn Law (Milchev, Bul); Experimentally investigating microfluidic penetration in microchannels (Pisignano, Ita).

The last issues has been discussed by; Elastic Turbulence and Mixing by Polymers in Micro-flows. (Steinberg, Isr); Flow of a polymer melt over a brush (Mueller, Ger)

Some fundamental open problems on foundation of Lattice Boltzmann have also been addressed in the two talks: The lattice Boltzmann hierarchy: Microflow, mixtures and renormalization (Karlin, CH); : Lattice Boltzmann beyond Navier-Stokes (Shan, USA);

A long discussion on follow-up research activities and/or collaborative actions or other specific outputs within or outside the frame of ESF (e.g. prepare the ground to develop a Forward Look, a Research Networking Programme, a EUROCORES proposal or an application to the EC Framework Programme) was held in the second day of the workshop. All participants agreed on the idea to try to develop a project to apply for a PhD network within the EU Fp7 program.

SCIENTIFIC CONTENT OF THE EVENT.

Andreotti discussed the nature of the dynamical wetting transitions. He presented experimental and theoretical results of the transition from static to dynamic interface profile due to the formation of a solitary wave in a Landau-Levich film.

Biben presented results on the Phase-field approach to the dynamics of a fluid near a structured wall. He showed how a phase-field model can investigate the static and the dynamical properties of a fluid near a textured wall. He showed that these models could help both theoreticians and experimentalists in testing or designing models or in understanding experiments.

Bocquet, presented theoretical and experimental results concerning possible strategies to displace fluids based on interfacial transport, such as electro-, diffusio- or thermo- phoresis.

Care described a two-component lattice Boltzmann scheme, designed to recover the continuum isothermal hydrodynamic description, in which a kinematic condition applies to the movement of the fluid-fluid interface. His method achieves significant interfacial density contrasts, very low microcurrents and a wide range of flow parameterizations. In particular the method is able to address problems of very low Reynolds number and large capillary number often associated with microfluidic flows. He also showed how the model can be adapted to recover multi-component Navier type boundary conditions and, thereby, be applied to dynamic wetting calculations.

Cieplak presented some numerical simulations based on Molecular dynamics of fluids in patterned nanochannels. In particular, both single phase and two-fluid case have been investigated. In the single-fluid case, the chemical patterning is shown to give rise to novel types of flows that involve spatial switching between Poiseuille and plug-flow behaviors. Geometrical indentations are found to affect the flow patterns less significantly than patterning of wettability. In the two-fluid case, such that the two immiscible fluids wet different patches of a chemically patterned channel, the velocity field is modulated in a way that is phase shifted relative to the single-fluid case.

Cottin-Bizonne studied the high slippage of liquids at walls, in terms of the use of gas as a lubricant – such as microbubbles trapped in superhydrophobic surfaces. In particular, she focused on the experimental characterizations of simple liquid flow slippage over super hydrophobic surfaces developed in the University of Lyon.

Craig presented recent advancements in measurement techniques of Boundary Slip in highly confined flows of Newtonian Liquids, showing how cantilever of different shape may leads to strongly different results.

Eggers presented an overview of recent theoretical and numerical advancements in understanding the formation of singularities in hydro dynamical systems.

Gonnella has presented a thermal Lattice Boltzmann Model for van der Waals fluids where the Prandtl number can be controlled independently on the viscosity. At second order of a Chapman-Enskog expansion, the model reproduces in the

continuum the hydrodynamic (mass, momentum and energy) equations with the stress terms as recently introduced by Onuki in Phys. Rev. Lett. vol. 94, 054501 (2005). He studied phase separation in a system, initially above the critical point, quenched by contact with external walls at temperature lower than the critical value. Harting studied via LBE the relevance of surface roughness when typical length scales of the system are comparable to the scale of the variations as it is the case in microfluidic setups. He found that the detected apparent slip is independent of the detailed boundary shape, but only given by the distribution of surface heights.

Jacqmin presented both analytical calculation, within lubrication approximation, and numerical results, within phase field model on the diffuse- and sharp-interface wetting failure. Karlin made a review talk on the lattice Boltzmann hierarchy. From microflow, to mixtures and renormalization He covered exact solutions in the microflow regime, realistic simulation of multicomponent mixture models, surface-based catalytic reactions, renormalization technique enabling simulation of large velocity sets on small lattices, and applications to modeling solid oxide fuel cells.

Lamura considered a single vesicle whose dynamics is described by Molecular Simulations, embedded in a solvent which is modeled at a mesoscopic level through Multi-Particle Collision Dynamics. He determined the root-mean-square of tilt angle, found to be in a remarkable agreement with the results of a recent experiment [V. Kantsler and V. Steinberg, Phys. Rev. Lett. 95, 258101 (2005).]

Milchev studied via Molecular Dynamics, the problem of Capillary Rise in Nanopores. He found good agreement with Lucas-Washburn Law if the slip length is taken into account.

Mueller studied the properties of a polymer brush in contact with a melt of identical chains under Couette and Poiseuille flow, using molecular dynamics simulations and dynamic single chain in mean field simulations. He also discussed the degree to which the flow can be described by a simple hydrodynamic boundary condition.

Pisignano presented some experimental investigation of microfluidic penetration in microchannels, showing the presence of long transient, unexpected by simple application of the Washburn-Lucas law.

Shan showed as recent progress in LBE provides an elegant and efficient way to include the contributions of higher hydrodynamic moments in computations. This is possible because the moment expansion scheme maps one-to-one to the discretization of the velocity space. He showed that the LB method can therefore be systematically extended to model flows of finite Knudsen numbers.

Steinberg showed that truly chaotic flow can be generated in smooth micro-flows at arbitrarily low Re , if a small amount of flexible polymers is added to the working liquid. This regime is termed "elastic turbulence". By using high molecular weight fluorescent passive tracers with different diffusion coefficients and by changing the fluid velocity he studied the dependence of a characteristic mixing length on the Peclet number, which controls the mixing efficiency. The role of the boundaries in the passive tracers distribution and the mixing length abnormal growth has been also quantitatively studied.

Tabeling presented an overview on some fundamental challenges faced by microfluidics. He described problems connected to multiple emulsions and he showed that by combining microfluidics and near field microscopy, it is possible to analyze flow motion within the first tens of nanometers from a wall.

Yeomans used the lattice Boltzmann algorithm as a tool to investigate the movement of drops on surfaces covered by an array of micron-sized posts, a geometry that leads to superhydrophobic behavior. She explored transitions between the fakir and collapsed states, contact angle hysteresis, and the way in which a drop moves across a superhydrophobic surface.

ASSESSMENTS OF THE RESULTS.

The workshop has certainly given an important contribution in the comprehension of basic properties of flows in microdevices, improved our knowledge on modelisation, and will certainly be helpful in order to further apply this knowledge to practical problems, as mixing properties and viscoelastic effects. In addition, during the workshop we have posed the basis for the creation of a common European group, gathering together the results from experiments and numerical simulations. For instance, a fruitful collaboration is already started between the researcher of the Rome group and the group of Dr. Andreotti in Paris, and between the researcher at CNR in Bari and Rome and the groups of Prof. Harting in Germany.

The possibility to establish a solid scientific network based on the funding of the EU FP7 has also been explored and will be pursued in the near future.

PROGRAMME

Thursday 27 September 2007

19:00 Welcome Aperitivo (Hotel Villa Vecchia)

20:00 Dinner (Hotel Villa Vecchia)

Friday 28 September 2007

08:45-09:00 **ESF Presentation** (Prof. Guazzelli and Prof. Beschkov)

09:00-09:45 **Eggers** (review) "Singularities in Microfluidics"

09:45-10:15 **Vinogradova** "Direct measurements of hydrophobic slippage using double-focus fluorescence cross-correlation". no-show

10:15-10:45 **Biben** "Phase-field approach to the dynamics of a fluid near a structured wall"

10:45-11:15 coffee break

11:15-11:45 **Bocquet** "Surface effects in fluid dynamics"

11:45-12:15 **Craig** "Measurement of Boundary Slip in highly confined flows of Newtonian Liquids"

12:15-14:00 Lunch (Villa Mondragone)

14:00-16:00 Visit to the archeological site "Barco Borghese"

16:00-16:30 **Cieplak** "Molecular dynamics of fluids in patterned nanochannels"

16:30-17:00 **Harting** "Roughness induced apparent slip in microchannel flows"

17:00-17:15 coffee break

17:15-17:45 **Care** "Modelling of dynamical wetting using the lattice Boltzmann method"

17:45-18:15 **Karlin** "The lattice Boltzmann hierarchy: Microflow, mixtures and renormalization"

18:15–19:15 informal discussion

20:00 Dinner (Hotel Villa Vecchia)

Saturday 29 September 2007

09:00-09:45 **Tabelling** (review) "Some fundamental challenges faced by microfluidics"

09:45-10:15 **Jacqmin** "Diffuse- and sharp-interface calculations of wetting success and failure"

10:15-10:45 **Yeomans** "Modelling drops on superhydrophobic surfaces"

10:45-11:15 coffee break

11:15-11:45 **Cottine-Bizonne** "Experimental studies of slippage of water past superhydrophobic surfaces"

11:45-12:15 **Steinberg** "Elastic Turbulence and Mixing by Polymers in Micro-flows"

12:15-14:00 Lunch (Villa Mondragone)

14:00-14:30 **Milchev** "Capillary Rise in Nanopores: Molecular Dynamics Evidence for the Lucas-Washburn Law"

14:30-15:00 **Pisignano** " Experimentally investigating microfluidic penetration in microchannels"

15:00-15:30 **Gonnella** "LBM simulations of phase separation in thermal nonideal fluids"

15:30-16:00 coffee break

16:00-16:30 **Shan** "Lattice Boltzmann beyond Navier-Stokes"

16:30-17:00 **Lamura** "Thermal and Hydrodynamic Effects on Closed Membranes in Shear Flow"

17:00-17:30 **Guazzelli**. "Falling clouds of particles in viscous fluids"

17:30–19:00 Discussion on follow-up research activities and/or collaborative actions or other specific outputs within or outside the frame of ESF (e.g. prepare the ground to develop a Forward Look, a Research Networking Programme, a EUROCORES proposal or an application to the EC Framework Programme)

20:00 Social Dinner (Castelgandolfo)

Sunday 30 September 2007

09:15-09:45 **Bechkov** "Some Hydrodynamic aspects of stability of colloidal systems"

09:45-10:15 **Mueller** "Flow of a polymer melt over a brush"

10:15-10:45 coffee break

10:45-11:00 **Kwok** "Electrokinetics in Micro and Nanofluidics", no-show. replaced by S. Succi.

11:00-11:30 **Sbragaglia** "Boundary Slip Phenomena in The Lattice Boltzmann Equation", no-show. replaced by L. Biferale

11:30-12:00 **Di Leonardo** "Light driven devices and sensors for microfluidics"

12:00–12:30 **Andreotti** "On the nature of the dynamical wetting transition"

13:00-14:00 Lunch (Villa Mondragone)

STATISTICAL INFORMATION ON PARTICIPANTS.

The workshop was supposed to be attended by 24 scientists plus the three local organisers plus a bunch of 3-4 local phd students. We have had only three no-show in the programme which have been replaced by presentations of two of the local organisers (Prof. Biferale spoke at the place of Dr. Sbragaglia and Prof. Succi spoke at the place of Prof. Kwok).

The two representatives of ESF, Prof. Guazzelli and Prof. Beschkov have also been kind enough to participate actively to the scientific works by presenting their contributions in the programme.

The participants (excluding ESF Representatives) came from 9 different countries (UK, 3; FR 5; AU 1; PL 1; DE 3; CH 1; US 2; IL 1; IT 7).

Gender representation was as follows: 22 M / 2 F.

FINAL LIST OF PARTICIPANTS

Bruno Andreotti andreotti@pmmh.espci.fr

PMMH

ESPCI, 10 rue Vauquelin , 75005 Paris, France

Thierry Biben thierry.biben@lpmcn.univ-lyon1.fr

Lyon I University

LPMCN, Université Claude Bernard Lyon 1

43 Boulevard du 11 novembre 1918 - 69622 Villeurbanne – France

Luca Biferale biferale@gmail.com

University of Tor Vergata

Via della Ricerca Scientifica 1, 00133

Roma, Italy

Lyderic Bocquet,

Université de Lyon - CNRS

LPMCN - Bat Brillouin - 43 bdd du 11 Nov 1918 69622 Villeurbanne, France

Chris Care C.M.Care@shu.ac.uk

Sheffield Hallam University

Materials and Engineering Research Institute, City Campus, Sheffield Hallam University,

Howard Street, Sheffield, S1 1WB, UK

Marek Cieplak mc@ifpan.edu.pl

Institute of Physics. Polish Academy of Science

Al. Lotnikow 32/46, 02-668 Warsaw, Poland

Cecile Cottin-Bizonne Cecile.Cottin-Bizonne@lpmcn.univ-lyon1.fr

LPMCN, CNRS Université Lyon1, France

Vince Craig vince.craig@anu.edu.au

Australian National University

Research School of Physical Sciences, Canberra ACT 0200 Australia

Roberto Di Leonardo roberto.dileonardo@phys.uniroma1.it

CNR-INFNM, Dip. Fisica, Univ. "Sapienza", p.le A. Moro 2, 00185 ROMA

Jens Eggers jens.eggers@bris.ac.uk
University of Bristol, UK

Giuseppe Gonnella Giuseppe.Gonnella@ba.infn.it
Dipartimento di Fisica - Universita' di Bari

Jens Harting j.harting@icp.uni-stuttgart.de
Institute of Computational Physics, University of Stuttgart
Pfaffenwaldring 27, D-70569 Stuttgart, Germany

David Jacqmin David.A.Jacqmin@nasa.gov
NASA Glenn Research Center
21000 Brook Park Road, Cleveland, Ohio, 44135 USA

Ilyia Karlin karlin@lav.mavt.ethz.ch
ETH Zurich, Switzerland

Antonio Lamura a.lamura@ba.iac.cnr.it
IAC CNR Bari

Andrey Milchev milchev@mail.uni-mainz.de
Bulgarian Academy of Sciences, Institute of Physical Chemistry
G. Bonchev Str. Block 11, 1113 Sofia, Bulgaria

Marcus Mueller mmueller@theorie.physik.uni-goettingen.de
Institut fuer Theoretische Physik, Georg-August Universitaet
Friedrich Hund Platz 1, D 37077 Goettingen, Germany

Dario Pisignano dario.pisignano@unile.it
National Nanotechnology Laboratory INFM-CNR
University of Lecce, via Arnesano 73100 – Lecce, Italy

Xiaowen Shan xiaowen@exa.com
Exa Corp.
3 Burlington Woods Drive, Burlington, MA, USA

Victor Steinberg victor.steinberg@weizmann.ac.il
Department of Physics of Complex Systems,
Weizmann Institute of Science Rehovot, 76100 Israel

Sauro Succi succi@iac.rm.cnr.it
CNR-IAC
Viale del Policlinico, Roma, Italy

Patrick Tabeling patrick.tabeling@espci.fr
ESPCI, 10 rue Vauquelin, 75231 Paris (France)

Federico Toschi succi@iac.rm.cnr.it
CNR-IAC
Viale del Policlinico, Roma, Italy

Julia Yeomans yeomans@thphys.ox.ac.uk
University of Oxford
Theoretical Physics, 1 Keble Road, Oxford, Ox1 3NP, UK