ERC Advanced Grant 2016
Research proposal [Part B2]
(not evaluated in Step 1)

Part B2: *The scientific proposal* (max. 15 pages)

Section A. State-of-the-art and objectives

A.1 State of the art and objectives

"Πάντα ῥεῖ, Everything flows", recites Heraclitus in 500 b.C., [KIRK10] but ... how? Despite the enormous progress in the basic understanding of the rheological properties of *soft glassy materials (SGM)*, more than two thousand years down the line, this question still stands with us [FERN16,COUS14]. Since they spend their entire lifetime far from equilibrium, the study of SGM calls for profound extensions of non-equilibrium thermodynamics [OETT95], capable of accounting for a series of anomalous effects, such as non-linear and non-local stress-strain relation, long-time relaxation, yield-stress behavior, hysteric ageing-rejuvenation response to external stimuli [BERH11,GOY08,SCHA07,SCHO16, SOLL97,SOLL12COHE13]. The above features play a crucial role in shaping up the SGM rheology, and most notably, its strong sensitivity to the initial and boundary conditions (preparation and load schedule). On the other hand, these anomalous features also offer tantalizing prospects of realizing new states of matter, which would not exist at thermodynamic equilibrium, with special properties which prove crucial for the design of new *soft mesoscale materials (SMM)*.

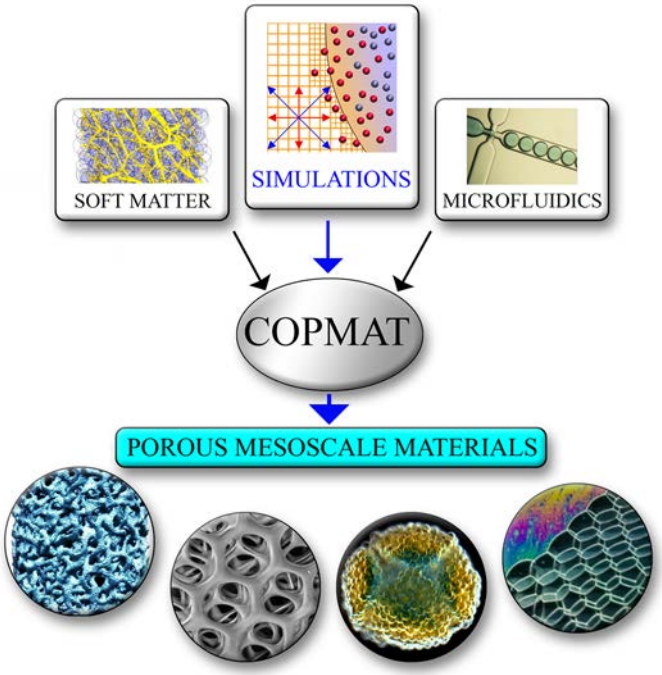

Figure 1: Schematic overview of COPMAT.

Here is where the tremendous progress in fundamental soft matter science [LISU12] ties in with the equally impressive advances of microfluidic science [WHIT06,NISI08]. The fundamental cornerstone of this connection is the dynamics of complex interfaces, which involves genuinely non-linear multiscale phenomena, ranging from the molecular size of close-contacts (breakup, merging and coalescence) to the full size of the devices, typically in the order of millimeters, spanning at least six orders of magnitude in space and no less than twice as many in time. ***The prime objective of COPMAT is to take up the formidable challenge raised by the above multiscale problem by performing full-scale simulation of microfluidic devices at nanometric resolution. This is set out to open up new transformative paths for the computational design and synthesis of a novel class of SMM, most notably Tunable Porous Materials (TPM) for bio-engineering applications.***

The interface dynamics is controlled by the competition/cooperation of multiple concurrent interactions; pressure, long-range hydrodynamics, near-contact capillary forces and viscous dissipation.

At low surface/volume ratios (low volume fraction of the dispersed phase, say oil in water for the case of emulsions) this competition can be treated by multiphase/component extensions of the Navier-Stokes equations of continuum mechanics. At high S/V's (low surface tension) however, different portions of the interface come in near-contact, thereby triggering short-scale capillary forces, which become dominant whenever the interface-interface separation, h~V/S, becomes comparable with the interface width w.

Formally, this regime is characterized by unitary Cahn number $Cn = w/h = Sw/V \sim 1$, marking the onset of complex *many-body* interactions [KRUG13].

Under these conditions, which are typical of many SMM, the micro and macrophysics aspects of the interface dynamics can no longer be separated and new theoretical and computational techniques are required. Many models have been developed in the last decades to address the above challenge [VOIG13, TRYG11,GOY08,COHE13,BALM14,BOUC09,BRAD09,BESS07,BOCQ09,KART09].

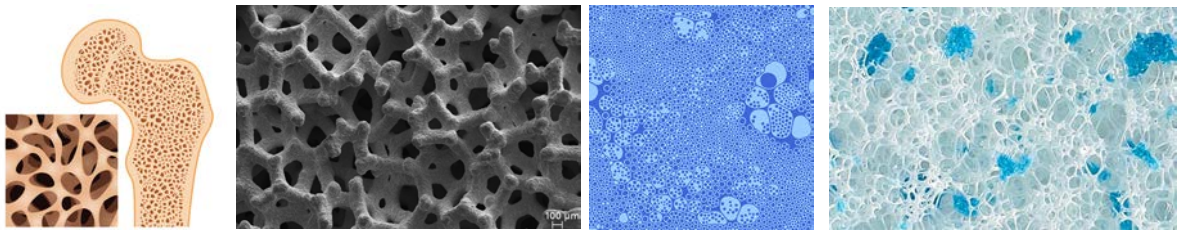

Figure 2: Examples of porous mesoscale materials: dry materials as bones, scaffolds (on left), porous soft materials as wet foams (on right).

However, to the best of the author's knowledge, all of them face with significant difficulties in providing direct access to fully three-dimensional and time-dependent flow configurations with highly complex interfacial dynamics, all the way from nano to millimeter scales [PROS07]. Indeed, in such regime a continuum approach based on extended hydrodynamic equations goes under question. At the same time, a fully microscopic approach, say molecular dynamics, appears computationally prohibitive when faced with the spacetime-scales of the engineering device. This "too small for continuum, too large for molecular dynamics" no-man's land, offers a unique opportunity for mesoscale modelling, aimed at combining the best of the two worlds. Indeed, mesoscale models have made proof or remarkable flexibility across a broad range of scales, from turbulence to biopolymer translocation [SUCC08,SUCC16]. However remarkable, such flexibility may not be sufficient to embrace the complexity of interfacial dynamics all the way from nano to millimeter scales. To this aim, a new class of multiscale computational models is required, capable of encompassing both the micro and macroscopic features of complex interface dynamics, including its interactions with the confining walls of the microfluidic device.

COPMAT *will address this challenge through the development of a unique class of multiphase models with enhanced multiscale capabilities for microfluidic design of new TPM. This goal shall be pursued by means of transformative combinations of a broad variety mesoscale models, mainly innovative variants of the Lattice Boltzmann (LB), as coupled to Immersed Boundary Methods (IBM), Dissipative Particle Dynamics (DPD), as well as completely new techniques, such as Dissipative Voronoi Dynamics (DVD), and Lattice Liouville equation (LLE) for the ab-initio calibration of LB pseudo-potentials (see Figure 1).* In the last decade, a whole array of efficient Lattice Boltzmann *schemes* [SUCB01, AIDUN10, BENZ92] *for multi-component fluid mixtures with competing short-range repulsion and mid-range attraction* [SBRA07] has been developed, which have proven capable of reproducing many of the anomalous signatures of SGM's, such as non-linear rheology, dynamic arrest, ageing and the dynamics of plastic events, under simple geometries [BENZ09,BENZ14].

On the other hand, the only way LB alone may eventually encompass six decades (mm to nm), is to enable it with *extreme grid refinement (XGR)* capabilities. By XGR, we imply at least 10 levels of locally doubled refinement, taking from microns to nanometers, including the possibility for the physical interface to straddle across different levels of refinement. The latter feature is crucial to resolve the near-contact interactions which play a key role on the mechanical properties of the material. This is an extremely challenging task, from both conceptual and technical standpoints, since it requires the continuity of kinetic *and* potential energy fluxes across the interfaces. *We plan to face this challenge through the resort to high-order lattices supporting multirange potentials beyond the second Brillouin region, supplemented with optimized equations of state geared towards the minimization of spurious currents* [YUAN06].

Besides a non-ideal equation of state and surface tension, such three-parameter models will deliver enhanced control over higher-order capillary forces, which are crucial to the complex interface dynamics.

We also plan off-line ab-initio calibration of the above LB pseudo-potentials by dedicated simulations of the *two-body lattice Liouville equation (LLE)* in micrometric regions of the flow around the interface. Residual spurious effects of the lattice discreteness on the fine scale structure of the near-contact interactions, shall be further minimized by coupling multirange LB to underlying DPD models with suitable potentials accounting for near-contact interactions [GROT97, ESPA95]. Both avenues above represent a major upgrade of mesoscale modeling at large.

In order to explore new design principles based on the synergy between plastic events and nano-corrugations, we also plan to couple LB with *Dissipative Voronoi Dynamics (DVD)*, a completely new technique for the early detection of plastic events. Further details on the main strengths of the COPMAT approach are given in section B1.

By leveraging the outstanding LB amenability to parallel computing [BERN13], COPMAT will give access to unprecedented full-scale simulations, permitting to: i) *Elaborate new rheological models, ii) Inspire new microfluidic experiments, iii) Inform and guide the design of microfluidic devices for the synthesis of new soft mesoscale materials.*

The result is a truly game-changing approach to the full-scale simulation and design of soft mesoscale materials via microfluidic devices, with potentially far-reaching implications beyond the lifespan of COPMAT.

A.2 Theoretical Objective: Microscopic foundations of soft glassy rheology

The details of SGM rheology are central to the design and production of TPM. SGM's exhibit non-trivial rheological properties, very distinct from the simple Newtonian behavior characterized by a linear relation between the applied stress and the resulting strain (see Figure 3). A broad class of SGM's obeys the so-called Herschel-Bulkley (HB) constitutive relation [COUS14,CHEN10]: $\sigma = \sigma_Y + AS^{\beta}$, where S is the strain rate (inverse time scale), β is a non-universal scaling exponent of the order 0.2-0.5, and A is a numerical prefactor marking the onset of non-linear behavior.

The simple case of Newtonian flows is recovered in the limit $\sigma_Y \to 0$ and $\beta \to 1$, yielding a constant dynamic permeability $\mu = \sigma/S$.

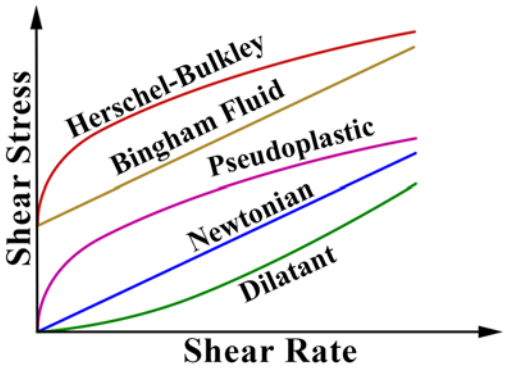

Figure 3: Different classes of rheological models.

Yield flow: The HB relation exhibits *yield* behavior, i.e. the material does not flow until the applied stress σ exceeds a minimum threshold σ_Y. This bears major consequences on the rheology of confined SGM because, in the presence of yield stress, any inhomogeneous flow configuration is potentially liable to intermittent stick-and-slip motion, characterized by local Flow-NoFlow transitions and viceversa (dynamic arrest/restart). In regions where $\sigma > \sigma_Y$, the fluid flows like a liquid, while in the regions where this condition is not met, the fluid remains at rest, like a solid [BENZ15].

Shear Banding: In actual experiments, characterized by *confined geometries*, the situation is however much more articulate; for instance, it is often observed that the shear rate $S(\vec{x})$ self-segregates in piecewise constant districts, corresponding to piecewise-linear distribution of the velocity field (see Figure 4), a phenomenon known as *shear-banding* [FIELD14].

Shear banding strongly affects the SGM rheology, hence the morpho-mechanical properties of the resulting SMM as well. Therefore, the conditions for its occurrence in actual microfluidic devices need to be analyzed in great detail.

Plastic Events: The relaxation towards equilibrium of most SGM's, proceeds through local topological rearrangements of the flow structure, called plastic events, which facilitate the transition from non-flowing to flowing states, as it typically occurs in proximity of yield-stress.

Plastic events release the structural constraints which hinder the relaxation to lower S/V configurations in a very short time lapse, i.e. with a strong degree of intermittency [BENZ14,SCHA07]. Among others, a popular approach to long-relaxation scenarios is provided by the Soft-Glass-Rheology model [SOLL97,SOLL12]. In this model, plastic events are viewed as non-thermally activated escapes from local "free-energy" traps. i.e. local minima of the energy configuration of the flow. The key point is that these configurational barriers (dynamic traps) are of the order of tens of $k_B T$, thus connotating plastic rearrangements as rare events in configuration space. In order to track the dynamics of such rare events in *topological rather than physical time*, a new class of multiscale methods will be developed, based on a two-level coupling between LB and Dissipative Voronoi Dynamics, to be detailed in section B.

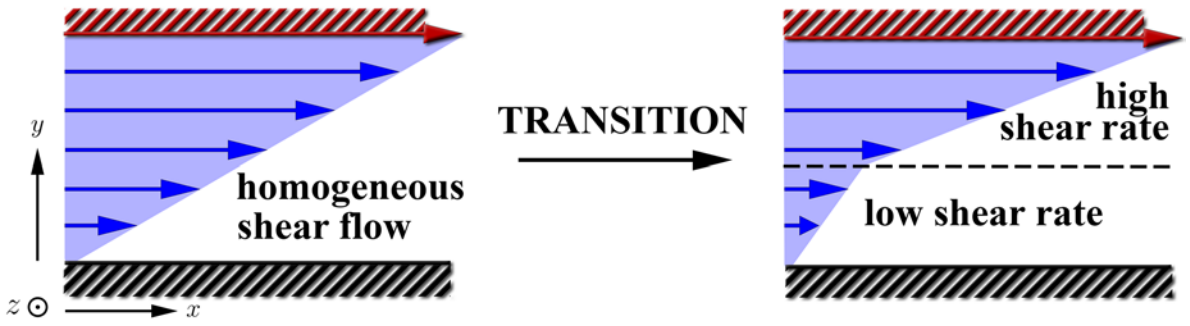

Figure 4: Linear Couette flow (left) versus "shear bands" (right).

Plastic events in the presence of nano-corrugations: We shall also investigate the potential synergy between the dynamics of plastic events and nano-corrugations of the confining wall. In particular, we shall explore the possibility of fine-tuning the nano-corrugations so as to increase the rate of plastic events,

thereby enhancing the overall flow of the material across the microfluidic device [SCAG15]. To this purpose, we plan to perform extensive series of very-long, high-resolution simulations of basic rheo-geometries, such as Couette and Poiseuille flows. The information delivered by such basic studies, i.e. effective dynamic rheological models will be incorporated within the full-scale simulations of the micro-reactors for the synthesis of the new SMM discussed in this project.

A.3 Application Objective: Computational design of new soft mesoscale materials

The search for new materials with mesoscale structure is a leit-motif of modern material science.

COPMAT will focus on three relevant classes of SMM: **Multi-jels, Trabecular Porous Media and Soft Mesoscale Molecules.** To this end, we shall perform **full-scale simulations** of microfluidic devices.

The notion of Full-Scale-Simulation:

For the sake of concreteness, we provide a few numbers which help clarifying the notion of "full-scale simulation". A very large scale LB simulation with ten billion sites, running over ten million timesteps can simulate the operation of a millimetric device over a time lapse of a few seconds, at a base resolution of about 100 nm. On a massively parallel Petaflop computer, such simulation is estimated to take about one-day elapsed time. By employing extreme grid-refinement and/or multiscale coupling close to interfaces, the local resolution can be pushed further down to 1 nm, *thus realizing the full-scale simulation of micro-engineering devices at nanometric resolution* (see Figure 5).

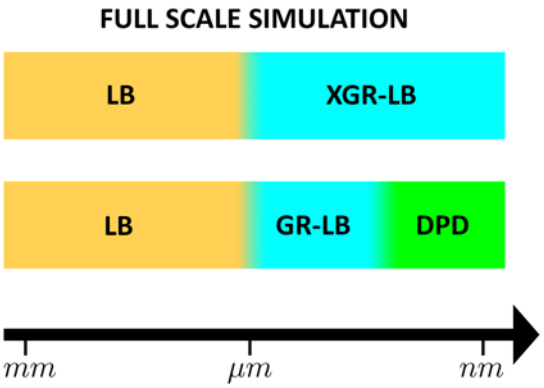

Figure 5: A scheme showing the strategies used in COPMAT: extreme grid-refinement (XGR-LB) and/or multiscale grid-refinement (GR-LB), coupled to dissipative particle dynamics (DPD).

A.3.1 Computational design of multi-jel materials

Bicontinuous interfacially jammed emulsion jels (bijels) are new multiphase soft materials in which two interpenetrating regions of immiscible liquids are stabilized by a jammed monolayer of colloidal particles, sitting at the interface between the two liquids (see Figure 6) [STRA05,JANS11]. Such materials were first predicted via (Lattice-Boltzmann) computer simulation and subsequently realized in the lab, with mixtures of water and lutidine (W/L) stabilized via silica colloids with near-equal affinity to both species. Bijels properties are predicted to be highly tunable in terms of the size and volume fraction of the solid particles and perhaps also their shape, say ellipsoids versus spheres, over a broad range of scales. For a colloidal volume fraction in the range $0.01 < \phi < 0.1$ and a radius $5nm < a < 5\mu m$, the stress modulus is predicted to vary in the range of 20 to 2×10^5 Pa, which is a very broad excursion for material design purposes. The unique architecture of W-L bijels can be exploited for template-based synthesis of hierarchically porous monoliths and composites with bicontinuous arrangement of the two phases at nano-micrometer scales.

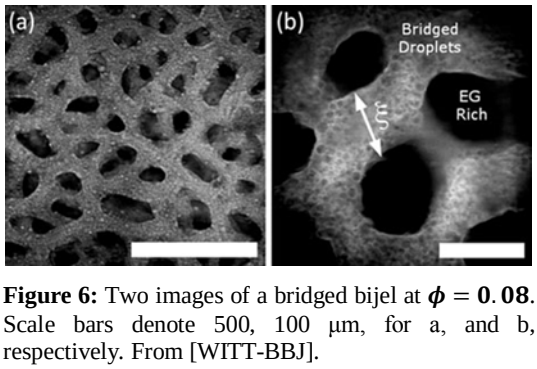

Figure 6: Two images of a bridged bijel at $\boldsymbol{\phi = 0.08}$. Scale bars denote 500, 100 μm, for a, and b, respectively. From [WITT-BBJ].

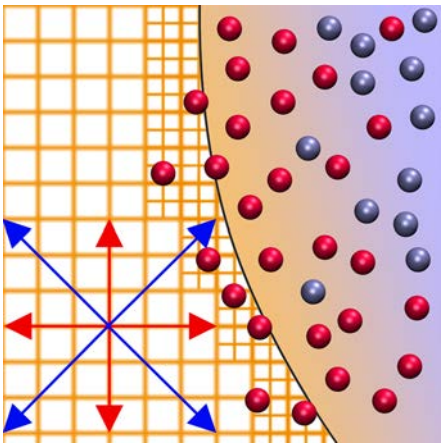

Figure 7: Sketch showing the coupling between multi-grid refinement LB solver and off-lattice solver for the colloid at the interface.

We plan to perform systematic studies of the morphological and mechanical properties of the bijel metastable structure, i.e. pore size and elasticity as a function of colloidal size and volume fraction. More specifically, we shall investigate the effects of the particle radius and volume fraction on the morphology, pore size distribution and resulting mechanical properties of the bijels for different types of motifs.

On the byside, we also plan to study Casimir effects due to fluctuations of the fluid concentration at the interface. Evidence of Casimir potentials of the order of $10-100\ k_BT$ has been reported in near-critical W-L bijels at distances of a few hundred nanometers for colloidal particles a few micron in radius [HERT08]. These may eventually affect the interface structure with very small colloids, say 10 nm in size. Likewise, it will be interesting to study the effects on the dynamics of the interface for the case of *polydispersed and/or nonspherical colloids*, which give raise to new materials with yet unknown properties. For many applications, say tissue engineering, it is imperative to access pore sizes above 100 μm, which appears problematic with standard bijels. This can be achieved by a variant of bijels, known as bridged bijels, in which one phase contains a network of colloidal-bridged droplets [WITT13] (see Figure 6). This dual morphology results from combined spinodal decomposition and nucleation and growth in a binary mixture containing neutrally wetting colloids with selective affinity for one liquid phase. Likewise bijels, the mechanical and morphological properties of bridged-bijels are highly sensitive to the physical-chemical properties and volume fractions of the colloidal particles.

All tasks above command a 10-100fold increase of the mesh resolution of the interface, such to secure a realistic scale separation between the colloidal radius and the interface width (see discussion on Cahn numbers in B1). This calls for a new generation of mesoscale schemes with extreme local grid refinement and/or multiscale coupling to particle methods for the colloids (see Figure 7).

A3.2 Computational design of trabecular porous media

We shall perform full-scale simulations of flow focusing microfluidic devices aimed at generating highly droplet configurations of O/W emulsions with crystal-like regularity (trabecular porous media) [HUER14,COST14,COST15,MALLO10,MARM09,BARB05,BARB09].

The prototypical device consists of a planar flow focusing circuit, integrated within a microchip about 1 mm in length and 300 microns in width (see Figure 8). The oil phase flows from the inlet chamber and mixes with the two streams of water from the top and bottom directions. Immediately downstream the channels which delivers the two phases, there is an orifice which forces the oil phase to inflate oil droplets in the outlet channel and release a droplet under the squeezing effects of the water cross-streams from above and below.

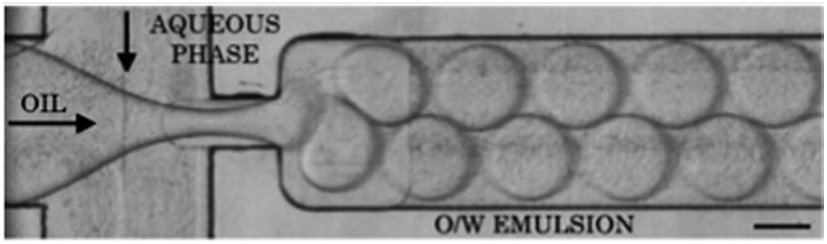

Figure 8: Optical micrograph of the flow focusing chip showing production of mono-disperse droplets. Scale bar is 100 μ [COST14].

As discussed in B1, the typical size of the device and droplets raise a mandatory call to multiscale modeling. The main goal of these simulations is to identify *optimal operational regimes capable of delivering droplet configurations of high regularity, both in size and connectivity* [GANA01,GARS04,GARS05]**.**

This responds to the need of delivering a uniform distribution of the chemical stimuli in micro-tissue engineering applications [LIN11,OH15,VILL13].

To date, the regularity is controlled via three main design parameters, i) Adjusting the flow rates of the two phases, ii) Scaling the dimensions of the channels, iii) Tuning the surfactant concentration in the aqueous solution. The COPMAT full-scale simulations will therefore focus on gaining quantitative insights into three scenarios above, namely:

Flow rates and Scale Dimensions; we shall perform an extensive set of simulations at different flow rates by changing the inlet velocity of the flowing phases and the size of the device.

Surfactant concentrations; same as above, with varying concentration of the surfactant, by changing the strength of intermolecular interactions which model the presence of the surfactant.

Nanopatterned microreactors; In addition, we shall also investigate a completely new design concept, based on the synergy between the dynamics of plastic events and nano-corrugations of the confining wall. This builds on very recent studies which point to the possibility of realizing super-hydrophobic regimes by properly tuning the geo-physico-chemical parameters of the corrugations, so as to induce a "resonance" with the typical scales of plastic rheology [TIAN16,SCAG15,DOLL15]. Such new designs may provide a

substantial enhancement of the reactor throughput, which is one the main constraints of current microfluidic design of SMM.

Experimental synthesis of trabecular porous media;

The fabrication of devices (chips) will require various types of micro/nanofabrication techniques, including *micro-milling, soft-lithography and hot embossing*.

When dealing with material synthesis processes, as in the case of trabecular porous media, the synthetized materials will be investigated from a materials science point of view, i.e. with the aim of correlating the chip geometry and process parameters with the material properties. The activity will therefore include morphological characterization (e.g. through micro-computerized tomography reconstructions), (micro)mechanical characterization, and more specific characterizations aimed at potential applications (e.g. for instance, scaffolds for tissue engineering). Most importantly, the experimental activities will provide an invaluable benchmark to test and improve the computational tools delivered by COPMAT. This activity will be carried out in strict cooperation with the experimental group at Campus Biomedic, University of Rome.

A3.3 Computational design of soft mesoscale molecules

As discussed in B1, double-droplets (DD) with soft deformable aqueous cores and oil shells offer the tantalizing opportunity of assembling a completely new class of materials with denser packing than the ones achievable by means of rigid colloidal particles [STEI12,CHEN11,HYVA08,ZERR08]. To this end, we shall simulate the microfluidic setup for production of double water-oil (W/O) droplets, as described in [GUZO15,GUZO13]. This consists of a T-junction with an inlet chamber filled with a third immiscible fluorocarbon (FC) phase (see Figure 9). Multiple double-droplets form with a hard-core aqueous bulk and an oil shell. Depending on the core (W)/shell(O) volume fraction (VF), $\phi = V_c/(V_c + V_s)$, different structural organizations are obtained. This information is summarized in the ϕ-N phase diagram.

For any number of droplets N, the packing/non-packing behavior is characterized in terms of our relevant VF's: $\phi_{max}(N) = Na^3/R_{min}(N)^3$, the maximum VF of hard spheres of radius a in a sphere of radius $R_{min}(N)$; $\phi_{pack}(N) = \phi_{max}(N)[1 + \Delta(\alpha, N)]$, the densest possible packing of hard spheres with contact angle alpha within a sphere of radius R_min(N). Due to the finite contact angle between aqueous cores, ϕ_{pack} exceeds ϕ_{max} by a small amount $\Delta(\alpha, N)$; ϕ_{cap} the VF at which the aqueous droplet exhibit a mild deformation, defined as less than 5% asphericity of the shell; ϕ_{chain} the VF's at which the double-droplets for linear chains due to capillary bridges between deformable shells.

Packing behavior is observed in the range $\phi_{pack} < \phi < \phi_{chain}$.

More precisely, for $\phi_{pack} < \phi < \phi_{cap}$., the droplets show weak deformations hence packing behavior not much dissimilar from hard spheres. However, in the range $\phi_{cap} < \phi < \phi_{chain}$, the substantial deformations trigger complex N-body interactions leading to a variety of metastable packings significantly denser than those available to hard spheres [MANO15,MANO03,ARKUS09,MENG10,MISZ11].

At a fundamental level, such structural richness owes to additional elastic interactions and energy barriers introduced by the deformability, which being larger than k_bT, do not yield to thermal relaxation.

As anticipated in B1, an accurate account of these highly complex interactions requires the development of an entire new array of computational methods, to be detailed in section B. The computational investigations will focus on major control aspects of the microfluidic design, namely:

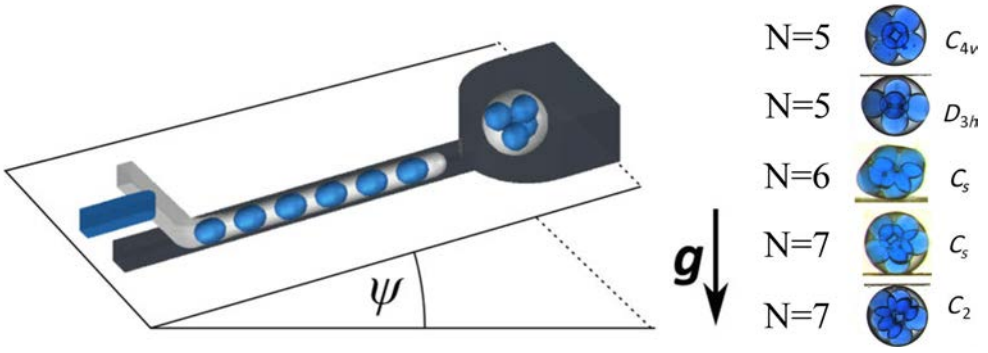

Figure 9: On left, the microfluidic device with two T junctions. On right, few examples of structures for several values of N, given N the number of aqueous droplets (blue) in oil (light grey) and fluorocarbon (third phase immiscible drawn in dark grey) [GUZO15].

Global geometry and tilt angle

At the moment, microfluidic experiments are performed on relatively simple T-junction based microchannels, with a tilt angle to gravity of about 40 degrees, corresponding to Bond numbers (gravity/surface tension) around 0.6. Increasing the Bond number through the tilt angle is expected to increase the number of droplets (we remind that the tilt angle controls the number of droplets independently of the volume fraction). However, excessive gravity can ruin the regularity of the droplet shape as well as of the patterns, whence the need of a parametric optimization, as well as exploration of different global geometries capable of attaining the highest values of N.

Long-range hydrodynamic interactions

Low-Reynolds hydrodynamics is characterized by long-range correlations, which significantly affect the motion of the various droplets, with a major impact on global morpho-rheological properties of the resulting SMM. This is particularly important for the case of micro and nano-confined flows, such as the ones occurring in COPMAT. The exploration of these effects is therefore crucial for optimal design purposes and again, may give rise to novel design geometries.

Core/Shell surface tension, S=sigmaW/SigmaO

This parameter shapes up the N-body interactions resulting from deformability.
Current studies are typically performed at S=4, but it is not known whether other values may lead to better performance. On intuitive grounds, one expects S larger than 1, for otherwise the core might loose stability towards the shell. On the other hand, S>>1 is not optimal either, for then deformability effects might be inhibited. Thus, optimization studies are in great demand.

Effects of nanocorrugations

As for the previous applications, we shall explore new microfluidic design concepts based on the synergy between nano-corrugations and plasticity.
Indeed, droplet-droplet interactions can be significantly altered by the presence of a solid wall, sometimes even in qualitative terms, i.e. change of sign of the interaction. Suitably engineered nano-corrugations might promote and enhance plastic events, thus facilitating the flow instead of hindering it (similar to super-hydrophobicity). Essentially, the proposed mechanism is as follows: untrapped droplets slide over the trapped ones, thereby experiencing less drag than they would from the solid wall. This is expected to occur whenever the size of the corrugations becomes comparable with the typical droplet size d, h/d ~1 [DOLL15,RAVE06,KUNE07].

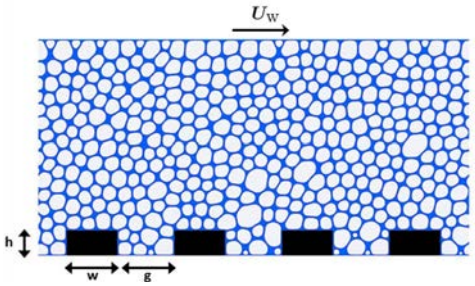

Figure 10: Sketch of a nano-corrugated set up facilitating plastic events, hence promoting enhanced fluid flow.

Section B. Methodology

COPMAT will be implemented through six major work packages (WP):

- *WP 0: Project Management;*
- *WP 1: Microscopic foundations of soft glassy rheology;*
- *WP 2: Computational design of new multi-jel materials;*
- *WP 3: Computational design of trabecular porous media;*
- *WP 4: Computational design of soft mesoscale molecules;*
- *WP 5: Dissemination, Communication and exploitation activities;*

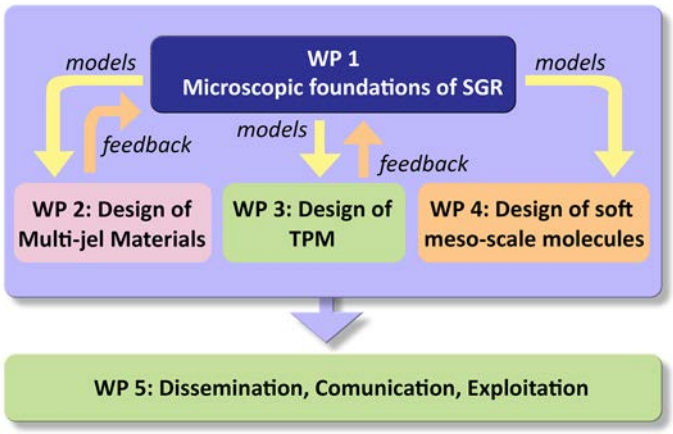

Figure 11: PERT diagram of the COPMAT project.

WP 0 is dedicated to the coordination and monitoring of the activities, the administrative and financial management. WP 1 provides the fundamental underpinning of COPMAT, by investigating fundamental aspects of soft glassy rheology. WP 2-3-4 deal with the implementation of basic rheological models within

real-life geometries relevant to actual microfluidic design for the experimental synthesis of the new materials. Finally, WP 5 is dedicated to dissemination activities.

The WPs 2-3-4 are conceptually connected through the common thread of soft glassy rheology (WP 1), and at the same time, largely independent in terms of their practical implementation. In WP 3, we plan to accomplish the concrete realization of trabecular porous media as suggested by the computational investigations. This latter task will be pursued in direct cooperation with the experimental team at the Biomedical Campus University in Rome. Finally, WP 5 is aimed at organizing several dissemination activities for the specialized community, communication activities for general public, and exploitation of main results obtained in COPMAT. In order to implement the above plan, we envisage to extend the current mesoscale computational technology along multifold directions:

1. *Multirange LB schemes with extreme grid-refinement,*
2. *LB/IBM schemes for multicomponent flows with colloidal particles*
3. *LB/DPD multiscale models for near-contact interactions,*
4. *LB/DVD multiscale coupling for plastic event detection*

Before delving into the details of the four main items above, a number of comments on the general merits of (lattice) kinetic theory are in order.

B.1: Why COPMAT?

Computational methods for complex flows is a very advanced and active subject, hence the reader may justly wonder why would COPMAT make the difference as compared to the current state of the art [FUST09]. In the sequel, we briefly highlight the peculiar strengths of the LB method, which, in our opinion, endow COPMAT with a unique angle of attack to the simulation of complex SGM flows.

The basic LB equation reads as follows:

$$f_i(x + c_i, t + 1) - f_i(x, t) = \omega\left(f_i^{eq} - f_i\right) + S_i$$

where f_i is the probability of finding a molecule at position x at time t with *discrete velocity* v_i, f_i^{eq} is a local equilibrium, ω a relaxation frequency fixing the fluid viscosity and S_i is a generic source of mass-momentum-energy reflecting the interactions of the fluid with its environment. With a suitable choice of the lattice symmetry, the above LB recovers the Navier-Stokes equations of continuum fluid mechanics and with further extensions, it describes a broad variety of complex flows, close and far from local equilibrium [LIB03,SUCC15,MONT15,AIDUN10,SUCC16, SUCB17].

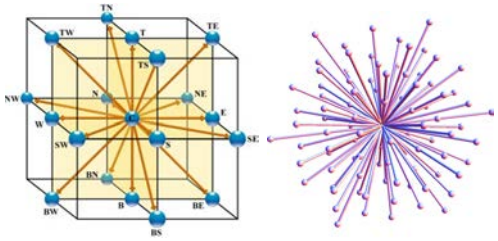

Figure 12: Standard D3Q19 and high-order D3Q93 lattices, with 19 and 93 discrete velocities, respectively [MONT11].

The LB features a number of very remarkable features which are unique to (lattice) kinetic theory:

1. *Streaming is exact:* LB information always travels along straight lines defined by the constant discrete velocities (Fig.12), regardless of the complexity in configuration space. This stands in marked contrast with the $u\nabla u$ term of the hydrodynamic representation, whereby the fluid moves its momentum along a trajectory defined by momentum itself. For complex flows, material lines become unwieldy complicated, leading to significant numerical difficulties especially in low-viscous regimes. Since the discrete velocities are constant, the LB streaming operator can be integrated *exactly*, offering a major simplification not only in low viscosity regimes but also for handling complex geometries, including fluid interfaces.
2. *Dissipation is emergent and Laplace-free:* The kinetic formalism keeps space and time on the same footing, both first order, and diffusion/dissipation emerge from relaxation of the momentum-flux tensor to its equilibrium value. As a result, no second order space derivative is ever needed, which is a major advantage for the computation of stresses near solid boundaries and multiscale interfaces.
3. *Pressure is local:* Pressure is available in space and time through a *local and linear* combination of the discrete Boltzmann populations, with no need of solving the Poisson equation to impose exact incompressibility. This leads to major computational savings, since the Poisson solver is one of the most expensive stages of hydrodynamic simulations. One might argue that artificial compressibility methods share the same bonus, but these methods are known to experience problems in tracking the correct flow dynamics.

4. *Outstanding amenability to multiscale and parallel computing:* Since LB information always travels along straight lines, highly efficient parallel implementations can be achieved also for the case of complex geometries and interfaces. Indeed, we are not aware of any other method capable of featuring nearly linear scalability on up to two million cores in realistically complex geometries (0.7 Petaflops multiscale hemodynamic simulations in human arteries) [BERN13].

Of course, the LB technique is not perfect. In particular, the physics of near-contact interfaces may be significantly affected by lattice discreteness. As mentioned before, COPMAT is poised to circumvent these weaknesses by deploying extreme grid refinement with a new class of multirange potentials on higher order lattices. Whenever residual artifacts show need for further reduction, multiscale coupling to mesoscale particle methods will be switched on.

B.2 Major extensions of mesoscale LB modeling of Soft Glassy Materials

LB schemes with non-ideal interactions have known an enormous boost for the numerical simulation of multiphase and multicomponent flows. However, they are also known to suffer a number of limitations which hinder a fully quantitative exploration of SGM's dynamics, primarily lack of resolution and spurious currents at the interface. These problems can be drastically reduced by increasing the resolution via local multiscale techniques and enhanced lattice connectivity (more discrete velocities). To this purpose, we shall develop *i) Multirange LB schemes with extreme grid refinement*, to achieve appropriate interface resolution; *ii) Multiscale LB/IBM schemes*, to deal with immersed bodies, such as colloids, surfactants and also deformable droplets, iii) *Multiscale LB/DPD* schemes for near-contact interactions, *iv) Multiscale LB/DVD schemes*, to accelerate the detection of rare events in plastic flows.
All of the above represent *transformative extensions* of the current mesoscale technology for complex moving states of matter.

B.2.1 Multirange LB scheme with extreme grid refinement

The prototypical LB scheme we have in mind is a multi-species kinetic equation of the form:

$$f_i^s(x + c_i, t + 1) - f_i^s(x, t) = \omega\left(f_i^{s,eq} - f_i^s\right) + S_i^s \ , \ s = 1, N$$

where N is the number of species and the source term describes multi-range interactions among the species, as well as statistical fluctuations whenever needed [DUN09,GROSS10].
Such generalized lattice kinetic equations can handle a very broad host of non-equilibrium problems and reinstate physical effects beyond the Boltzmann picture. i.e. strong interactions, non-diluteness, space-time non-locality and fluctuations [SHAN93,LADD94]. In particular, a proper fine tuning of the interaction parameters permits to achieve the main ingredients of frustration, i.e. small surface tension and positive disjoining pressure [BENZ16,BENZ13,SBRA12].The description of many-body interactions via LB pseudo-potentials is very effective in the bulk phases, but goes under question in the vicinity of strong non-equilibrium interfaces, especially in connection with non-negligible Cahn numbers (ratio of interface separation to interface width) which interfere with lattice discreteness. This is where (extreme) grid refinement will take stage [FILI98, SUCC01] (***milestones M.1.1.1*** and ***M.1.1.2*** of ***WP 1*** reported in ***Section* B.3**). The problem is fairly challenging due to the need of securing continuity of the fluxes of *both kinetic and potential energy* across the physical and multigrid interfaces [FAKH16, YU09,FILI98,SUCC01]. Grid refinement will be implemented on a new class of multirange pseudo-potentials extending beyond current implementations (see Figure 13), which are limited to second Brillouin regions (2-belt) at most [FALC11].
In particular, the implementation of 3-belt pseudo-potentials on higher-order lattices achieving up to 8th order isotropy, will allow a better control of short-range capillary interactions. These pseudo-potentials will be tested first on an empirical basis, i. e. by calibrating their strengths ex-post via dedicated simulations aimed at measuring capillary forces under *controlled near-contact conditions*. On a more fundamental basis, we also plan to map them out using ab-initio simulations of a two-body lattice Liouville equation. The computational cost is formidable, since the two-body distribution lives in a 12-dimensional space (plus time), hence it must be restricted to sub-micrometric regions.
This will permit the *ab-initio calibration of effective pseudo-potentials*, to be used in the actual full-scale simulations, similarly to consolidated pseudo-potential practices in computational chemistry.

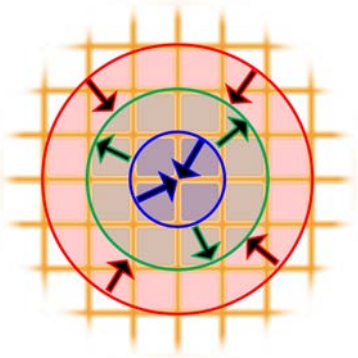

Figure 13: Conceptual scheme of the LB pseudo-potential extending to the third Brillouin region in 2d. We highlight three shells, two attractive (blue and red), and one repulsive (green).

B2.2 LB/IBM

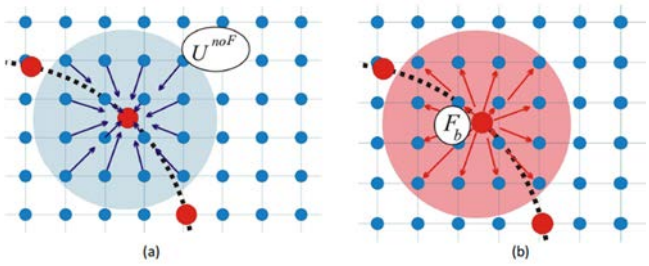

Figure 14: The basic IBM interpolations: the smoothed particle imports the velocity from the fluid sites (left) and exports the force back (right). [AMIR14]

The basic idea of the LB/IBM multiscale coupling (***milestone M2.1.1*** of ***WP 2***) is to treat the fluid (solvent) in Eulerian form via LB, and the immersed body as an off-grid Lagrangian structure (rigid colloid and eventually aslo deformable droplets) moving along with the fluid. The main appeal of this scheme is the dynamic adaptivity of the IBM method which permits to save on the depth of LB refinement [ROS13, FENG04]. On the IBM side, we plan to employ high order splines (smoothed particles) with at least four grid points per particle diameter. This is known to yield substantial overheads in the LB/IBM/LB handshaking procedure, but the payoff in terms of smoothness on the interaction justifies the computational cost.

B.2.3 LB/DPD

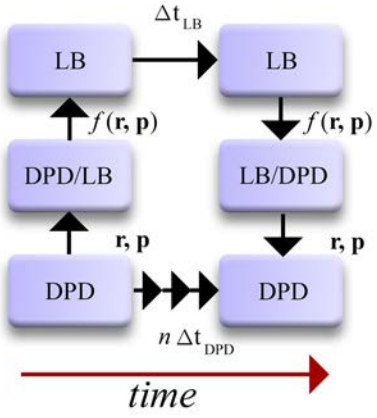

Figure 15: Conceptual scheme of the LB/DPD multiscale scheme. Both coexist around the interface, and exchange the corresponding flow descriptors, namely the discrete distributions f_i and the discrete positions and momenta (R,V) for LB and DPD, respectively. By construction, DPD ticks on a shorter time-scale than LB.

Dissipative Particle Dynamics is a major mesoscale particle method, which has gained significant visibility in the last decades, mostly for the simulation of low-Reynolds complex micro and nanoflows. One of its major merits is the capability of including thermal fluctuations in a thermodynamically consistent way, through compliance with the Fluctuation-Dissipation theorem [ESPA95]. Another plus of DPD is its formal resemblance to molecular dynamics. As a result, DPD can be employed as a meso-micro solver to resolve the fine scales, below microns, where LB may eventually suffer the effects of lattice artifacts. In order to resolve near-contact interactions (***milestone M3.1.1*** of ***WP 3***), we plan to keep a dynamic DPD "halo" around the diffuse interface (5-10 LB units thick). Such halo coexists with the LB lattice, its role being to describe the near-contact many-body interactions which are potentially distorted by lattice artifacts. Suitable handshaking procedures will be set up at both internal and external sides of the droplet to secure continuity of the thermo-hydrodynamic variables, as well as their corresponding fluxes. Similar procedures have been recently developed by the PI and collaborators for the multiscale coupling of LB with Direct Simulation Monte Carlo [DIST16]. The LB/DPD case is more challenging because the interface moves all the time. Besides, one must secure the consistency of the LB pseudo-potentials with the DPD soft-core potentials, which is a totally unexplored issue. We anticipate significant progress in assessing how close DPD can be brought to MD without losing its computational edge versus purely atomistic methods.

B.2.4 LB/DVD

Tracking the dynamics of plastic events in physical time is extremely time consuming, for they do not follow a regular schedule in physical time, but rather occur in highly intermittent spikes. To handle this highly intermittent dynamics, we plan to couple the LB simulator to a coarse-grained dissipative Voronoi dynamics (DVD) solver [FLEK99] (***milestone M4.1.1*** of ***WP 4***).

More precisely, the LB configuration will be mapped into a corresponding coarse-grained Voronoi representation (see Figure 16). Each Voronoi cell contains thousands of LB cells (in D=3), and it is characterized by its mass M_v, Position $\vec{R}_v$ and velocity $\vec{V}_v$. Therefore, upon developing appropriate potentials and dissipative forces, the DVD system can be evolved in time on its own, like DPD, this time however on a longer time-scale than the underlying LB [SCAG16].

This will help bridging the gap between the physical time of the simulation and the topological time of the plastic dynamics. As in any concurrent scheme, the major source of uncertainty/inaccuracy is the reconstruction of the information lost in projecting the fine-grained LB distribution onto of the coarse-grain DVD set of variables. This requires intensive sampling of the DVD positions and velocities, so as to produce a corresponding distribution function, to be subsequently constrained to the desired LB set of lattice discrete velocities [DIST16]. Should this face with unexpected problems we plan to develop a new class of LB schemes with *history-dependent potentials* which, in the spirit of metadynamics [LAI02], prevent the system from visiting the same state twice.

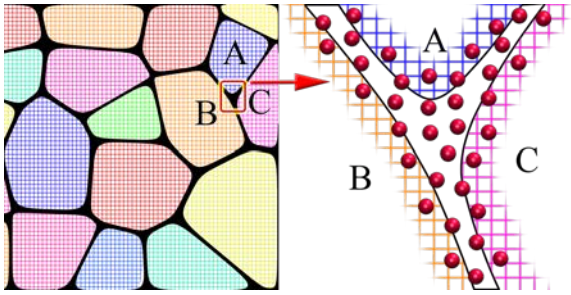

Figure 16: On left, Voronoi analysis of interfaces between immiscible fluids. On right, discrete representation (red particles) of the complex interface reported on left between three Voronoi cells (labeled A, B and C) integrated by dissipative particle method coupled to LB solver (represented as square motif).

B 2.5 Experimental synthesis of tunable porous media

One of the highlights of COPMAT is the realization of the in-silico models into real-world experiments. Besides providing an experimental validation of the results of the simulation environment developed in COPMAT, these activities will also serve as a demonstrator of the impact of computationally-informed chip design in real-world applications. Although all WPs 1-4 are potentially liable to experimental realization, we focus essentially on the synthesis of tunable porous media (***WP 3***). Besides meeting the goal of synthesizing TPMs, this choice reflects the natural resonance between the basic physics (interfaces, walls, nano-corrugations, multicomponent-multiphase systems, exotic rheologies) and the broad array of techniques developed across WPs 1-4.

The fabrication of devices (chips) will require various types of micro/nanofabrication techniques, including *micro-milling, soft-lithography and hot embossing*, and it will be carried out in collaboration with Dr. Alberto Rainer at Biomedical Campus University of Rome.

When dealing with material synthesis processes, as in the case of trabecular porous media, the synthetized materials will be investigated from a materials science point of view, i.e. with the aim of correlating the chip geometry and process parameters with the material properties (***milestone M3.2.3*** of ***WP 3***). Most importantly, the experimental activities will provide a valuable benchmark to test and improve the computational tools delivered by COPMAT.

B.3 Summary of Deliverables, Milestones, Gains , Risks and metric of success

Summarizing, COPMAT will deliver: *i) a deeper understanding of the microscopic foundations of the structural properties and local/global rheology of soft-glassy materials under geometric conditions of experimental and engineering interest, ii) provide extensive computer explorations of the optimal design parameters of current microfluidic devices for the synthesis of new SMM, iii) test innovative microfluidic design principles for the synthesis of new SMM.*

Further, new codes and computational tools which will be made available to the community under GNU GPL license.

COPMAT is organized in six main work packages (WPs), each targeted to a well-defined innovative scientific task. The whole work plan is reported in the Gantt Chart of Figure 17.

In particular, COPMAT articulates as follows (the number of man months required to carry out the work is reported in parenthesis for each WP):

- WP 0 “Project Management” is related to the coordination and monitoring of the activities, the administrative and financial management, the coordination of the reporting and deliverables production, the management of the knowledge generated in order to promote and facilitate the project activities. The PI, supported by the Research Coordination Office and Technology Transfer at IAC-CNR, will coordinate activities, periodic reporting and will organize, implement and follow up a kick-off meeting and periodic check-point meetings.
- WP 1 “Microscopic foundations of SGR” (128 man months) contains two deliverables (labeled D) and five milestones (labeled M). ***D1.1:*** *Basic multirange LB solver with extreme grid refinement-XGR (delivered at 24° month);* ***D1.2:*** *Rheological models for SGR (delivered at 36° month);* ***M.1.1.1:*** *XGR with standard LB lattices;* ***M1.1.2:*** *XGR with higher-order lattices;* ***M1.2.1:*** *Role of yield-stress and*

shear banding on the rheology of SGM ; ***M1.2.2:*** *Role of plastic events on the rheology of SGM;* ***M1.2.3:*** *Role of the interactions between plastic events and nano-corrugations on the rheology of SGM.*

- WP 2 "Computational design of multi-jel materials" (78 man months) includes two deliverables and three milestones. ***D2.1****: Multirange LB/IBM open source code (delivered at 30° month);* ***D2.2****: Assessment of mechanical properties of the multijel materials (delivered at 42° month);* ***M2.1.1:*** *Development of grid refined multirange LB-IBM solvers;* ***M2.2.1****: Bijel characterization;* ***M2.2.2:*** *Design of the microfluidic devices for bijel synthesis.*
- WP 3 "Computational design of trabecular porous media" (124 man months), probably the most demanding, will last four years, involving two deliverables and five milestones. ***D3.1:*** *Multiscale LB/DPD open-source code (delivered at 36° month);* ***D3.2:*** *Design specifications for the synthesis of trabecular porous media (delivered at 60° month);* ***M3.1.1:*** *Development of multiscale LB/DPD solvers;* ***M3.2.1:*** *Optimization of microfluidic device with smooth walls;* ***M3.2.2:*** *Optimization of the microfluidic device with nano-corrugations;* ***M3.2.3:*** *Experimental realization in collaboration with Biomedical Campus University of Rome.*
- WP 4 "Computational design of soft-molecules" (78 man months) includes two deliverables and three milestones. ***D4.1:*** *Multiscale LB/DVD open-source software (delivered at 42° month);* ***D4.2:*** *Design specifications for the synthesis of soft meso molecules (delivered at 60° month);* ***M4.1.1:*** *Development of LB/DVD solver;* ***M4.2.1:*** *Global geometrical design optimization;* ***M4.2.2:*** *Global optimization, including details of nano-corrugations.*
- WP 5 "Dissemination communication and exploitation activities". This WP is aimed at organizing several *dissemination* activities for the specialized community, *communication* activities for general public, and *exploitation* of main results obtained in COPMAT. To this purpose the *dissemination* plan includes three main events: an initial kick-off event (deliverable ***D5.1*** in Figure 17), a workshop at about 2 years from completion (***D5.3***), and a final event (***D5.5***) at the end of the project. Further, the participation to high level conferences worldwide will be a main goal of COPMAT. I also plan the realization of a **Project Website** in order to secure the highest visibility to COPMAT. Furthermore, publications in open access reviews will be kept on focus, in order to ensure a widespread dissemination of the results obtained in COPMAT and provide awareness of its benefits to the scientific community. Finally, I plan to organize meetings with private companies in the bio-medical engineering sector, in cooperation with the Biomedical Campus University of Rome (deliverables ***D5.2*** and ***D5.4***). In the context of *communication* activities, I plan a continued presence at major public events on science and society, as well as a continued presence at major public events on science and society, such as TED talks. I also plan to reach public education institutions through a concerted collaboration with Zanichelli, the main italian scientific Editor (see youtube "La scienza a scuola", in

month	1-6	7-12	13-18	19-24	25-30	31-36	37-42	43-48	49-54	55-60
WP 0	Project management									
WP 1	Microscopic foundations of soft glassy rheology									
Milestones		M1.1.1	M1.2.1	M1.1.2	M1.2.2	M1.2.3				
Deliverables				D1.1		D1.2				
WP 2		design of new multi-jel materials								
Milestones			M2.1.1	M2.1.1		M2.2.2				
Deliverables					D2.1		D2.2			
WP 3			design of trabecular porous media							
Milestones					M3.1.1	M3.2.1		M3.2.2		M3.2.3
Deliverables						D3.1				D3.2
WP 4					design of soft mesoscale molecules					
Milestones						M4.1.1	M4.2.1		M4.2.2	
Deliverables							D4.1			D4.2
WP 5	Dissemination communication and exploitation activities									
Deliverables		D5.1		D5.2		D5.3		D5.4		D5.5

Figure 17: Gantt Chart.

Italian). I will take care of IPR protection and coordinate the scientific activities by also evaluating different channels for *exploitation*. In particular, access rights to codes and computational tools developed in COPMAT will be granted to the community under GNU GPL license. Further, *exploitation* of results obtained in COPMAT will be promoted through the planned meetings (***D5.2*** and ***D5.4***) with private companies, in order to foster academia-industry collaborations, including the possibility of start-up companies.

Feasibility and Risks: COPMAT is poised to simulate complex flows over six spatial decades, a task which is inherently high-risk, as it is going to stretch multiscale modelling of complex flow beyond its current limits. Feasibility is nevertheless protected by the high degree of modularity of the COPMAT structure, which builds upon a number of alternative/complementary tasks, each of which can be operated nearly independently, thus making the risk of global failure a pretty remote event. Nonetheless, risks have been *estimated* according to the proposed risk matrix (see Figure 18), on the basis of the standard formula: risk = severity × likelihood. These are qualitatively reported in the table below.

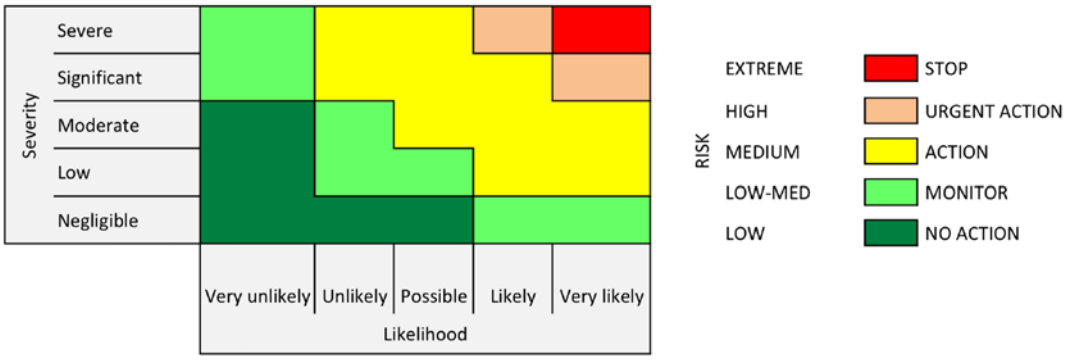

Figure 18: Risk matrix adopted for risk identification.

Description of risk	***WP***	***Proposed risk-mitigation measures***
Unsatisfactory performance of multirange LB solver with XGR (index: LOW-MED)	WP 1	In case of low performances, I plan to resort to the multiphysics code MUPHY [BERN09] (that I contributed to develop) which features outstanding level of parallel performances.
Low performance of XGR multirange for investigating plastic events effects on SGM rheology (index: LOW-MED)	WP 2	A highly parallel implementation in CUDA programming language of the algorithm could boost its performances. Further, DVD/LB scheme could be used as alternative in order to speed up the simulation.
Low reliability of pseudo potentials involved in DPD/LB scheme (index: MEDIUM)	WP 3	The event is possible, but its severity is moderate. In this case, I plan to use the two-body Lattice Liouville solver which permits an *ab-initio* calibration of the pseudo-potentials.
Technical hurdles in developing the DVD/LB scheme (index: MEDIUM)	WP 4	This risk is comparatively high, but of moderate severity. As an alternative, I plan to explore LB schemes with *history-dependent potentials.*

Potential risks factors in COPMAT are mainly related to simulation techniques. Since we have catered for several alternative/complementary approaches, **global failure is to be regarded as a highly unlikely event**.

Competence: My record shows that, in three decades of competitive research, I have been able to initiate and handle a very broad spectrum of complex flow problems, ranging from thermonuclear plasmas, fluid turbulence, micro and nanoflows, as well as quantum-relativistic fluids, often trailblazing new original approaches and research directions. In the course of this extensive activity, I have developed a detailed command at a broad array of computational techniques, from Montecarlo methods and finite-elements, to spectral methods and finite-volumes for macro fluids, to Molecular Dynamics for micro and nano-

hydrodynamics. However, my name is mostly associated with the Lattice Boltzmann method, a very successful method for fluids and beyond, which I have contributed to develop from the early days of its very inception, all the way up to the advanced applications we witness today, across virtually all walks of modern fluid dynamics and allied disciplines. As a result, I feel like I can offer unique credentials for the success of COPMAT.

Metric of success: COPMAT success will be measured by its effectiveness in inspiring and actually guiding the experimental design of microfluidic devices for the synthesis of a new generation porous materials for bioengineering applications. To emphasize the crucial value we place on this engineering goal, COPMAT explicitly caters for the experimental realization of the most promising innovative design concepts emerging from the full-scale simulations conducted within the project.

B.3.1 The COPMAT legacy

The full-scale simulation strategy developed within COPMAT is expected to establish a game-changing computational design paradigm, extending far beyond the 5 years horizon of the project.
As computers and algorithms get faster and better, the paradigm of full-scale computational design of new materials at molecular resolution will become increasingly accessible to routine operation for future generations of scientists in Academia and Industry, making computer simulation an even closer ally of experimental and theoretical research. *Why me?* My record shows that in about three decades of active research, I have been able to successfully initiate and handle a very broad spectrum of complex flow problems, ranging from thermonuclear plasmas, fluid turbulence, micro and nanoflows and lately even quantum-relativistic problems. In particular my trailblazing contributions and continued innovations to the Lattice Boltzmann method over the years are widely recognized by scientific community. As a result, I feel like I can offer unique credentials to make of COPMAT a prominent success story of European science.

Section C. Resources

C.1 Justification of the Resources

COPMAT requires substantial funding to build a dedicated team of computational scientists working under my coordination, which will complement the competences of my group in Rome. I plan to employ three postdocs (€ 252,000 for 108 man-months), two for the theoretical tasks, and one for the experimental part (milestone M3.2.3 in WP 3) to work in strict collaboration with Dr. Alberto Rainer under my supervision. Finally, a senior postdoc (€ 160,000 for 60 man-months) will be hired for five years to supervise all tasks in detail. From my institution, IAC, I will involve in COPMAT the following permanent researchers: Dr. Roberto Natalini director of IAC (€ 55,684 for 5 man-months), and Dr. Giuseppe Pontrelli (€ 71,748 for 10 man-months) (for a total € 127,432 as "Other Permanent IAC personnel" in the table below).
Through this Grant, ***a new generation of young scientists will be trained***. Indeed, I plan to open five Ph.D. scholarships (€ 16,523 per year / per Ph.D. scholarship), two for WP 1, one for each remaining WPs. I regard the training of the students as one of my central duties and I will spend an intense effort to make sure that they complete their tasks within three years time-frame, in line with the Italian law. Since the "Consiglio Nazionale delle Ricerche-IAC" cannot directly issue a Ph.D. certificate, the Ph.D. scholarships will be delivered in collaboration with the University of Rome "La Sapienza", where I am a member of the Ph.D. board. I will devote the overwhelming share of my research activity to this project, corresponding to 75% of my working time (€ 394,760 for 45 man-months), because of teaching duties at Harvard. Should COPMAT be granted, I will negotiate my teaching terms accordingly. The travel costs, estimated in 80,000 EUR, are justified by the **high number of international conferences**, where the results will be presented. I plan at least six conferences per year. I estimate 50,000 EUR for publications, with an average cost of 2,000 EUR per Open Access publication, with on average 5 publications per year. Publication on open access reviews will ensure a widespread dissemination of the results obtained in COPMAT.

In "other goods and services", I estimate 5,000 EUR for an Audit Certificate, 20,000 EUR as costs for conference fees, and 52,000 EUR for the organization of dissemination events planned in WP 5, for a total of 77,000 EUR. In particular, I estimate 5,000 EUR for the organization of dissemination events and the kick-off meeting (***D5.1***, ***D5.2*** and ***D5.4*** in Figure 17), 2,000 EUR for catering services of the events, 20,000 EUR for each remaining workshops (***D5.3*** and ***D5.5***, 40,000 EUR in total), and 5,000 EUR for the realization of the Project Website.

For equipment, I plan to spend 15,000 EUR for a workstation, which will be used to store and backup the computational data produced in COPMAT. The necessary computational infrastructure will be secured via multiple sources; first a GPU cluster of 64 Nvidia-Tesla K80 cards, 4992 SMX CUDA cores each, for a total of 319,488 CUDA cores and 1,536 Terabytes located at IAC-CNR (the largest Italian Institute of Applied Math). In addition, I plan to access the computational facilities of the Consorzio Interuniversitario

per il Calcolo Automatico d'Italia-CINECA, IAC-CNR is a member of. In particular, I estimate 100,000 EUR to buy part of the required computational time (100,000 EUR as subcontracting cost, € 0.05 per CPU hour corresponding to two millions of CPU hours). Finally, following a consolidated and successful practice, we plan to apply for PRACE grants.

For the experimental part of WP 3 (milestone ***M3.2.3***), I estimate in 25,000 EUR the subcontracting costs related to the activity conducted at the laboratory of microfluidics of Biomedical Campus University of Rome (costs for the fabrication of devices as microfluidic chips).

Cost Category			**Total in Euro**
Direct Costs	**Personnel**	PI	394,760
		1 Senior Postdoc	160,000
		3 Postdocs	252,000
		5 Ph.D. Students	247,856
		Other Permanent IAC personnel (except the PI)	127,432
	i. Total Direct costs for Personnel (in Euro)		1,182,048
	Travel		80,000
	Equipment		15,000
	Other goods and services	Consumables	0
		Publications (Open Access fees), etc.	50,000
		Other (Audit Certificate, dissemination events)	77,000
	ii. Total Other Direct Costs (in Euro)		222,000
A – Total Direct Costs (i + ii) (in Euro)			1,404,048
B – Indirect Costs (overheads) 25% of Direct Costs (in Euro)			351,012
C1 – Subcontracting Costs (no overheads) (in Euro)			125,000
C2 – Other Direct Costs with no overheads (in Euro)			0
Total Estimated Eligible Costs (A + B + C) (in Euro)			1,880,060
Total Requested Grant (in Euro)			1,880,060

Please indicate the duration of the project in months:	**60**
Please indicate the % of working time the PI dedicates to the project over the period of the grant:	**75%**
Please indicate the % of working time the PI spends in an EU Member State or Associated Country over the period of the grant:	**80%**

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