Ministero dell'Istruzione, dell'Università e della Ricerca
Dipartimento per l'Università, l'Alta Formazione Artistica, Musicale e Coreutica e per la Ricerca
Direzione Generale per il Coordinamento e lo Sviluppo della ricerca

Programma "SIR"
Decreto del 23 gennaio 2014 prot. n. 197
Protocollo: RBSI14R9ZX

A - ADMINISTRATIVE FORM

1 - Proposal number
RBSI14R9ZX

2 - Proposal acronym
NOVUSACTUS

3 - Proposal title
NOVel approaches and nUmerical methodS for ACTive flUidS

4 - Duration of the project
36 months

A.1 - PRINCIPAL INVESTIGATOR AND SUMMARY OF THE RESEARCH

1 - Principal Investigator

Family name	SCAGLIARINI
First name	Andrea
Fiscal code	SCGNDR81R19H501G
Nationality	ITALY
Date of birth	19/10/1981
City of birth	ROMA
Country of birth	ITALY

City of residence	Velletri
Country of residence	ITALY
Address	Via Croce 29
Postal code	00049
Phone number	069638752
Mobile number	3395723855
E-mail address	scagliarini@roma2.infn.it

2 - Date of first PhD
PhD awarded on the 28 of February 2011

3 - Publication list and brief track-record
scagliarini_publications.pdf - file with the LIST of your publications (only publications in peer-reviewed journals, conferences, symposia and workshops, etc)
scagliarini_track_record.pdf - file with a brief track-record (1 page maximum)

4 - Tutor of PhD
Family name Biferale
First name Luca

5 - Publication produced without the participation of tutor specified in the previous paragraph

A. Scagliarini,
"Geometric properties of particle trajectories in turbulent flows",
Journal of Turbulence 12, N25 (2011).
ISSN: 1468-5248

6 - Statement on extension of eligibility period
No, I declare not to take advantage of the extension of periods of eligibility

7 - Statement on the employment status
No, I declare not to be permanent employee of the host institution

8 - Primary ERC sector
PE3 - Condensed Matter Physics: Structure, electronic properties, fluids, nanosciences, biophysics

9 - Secondary ERC sector

10 - Primary ERC sub-sector
PE3_13 - Structure and dynamics of disordered systems: soft matter (gels, colloids, liquid crystals...), glasses, defects…

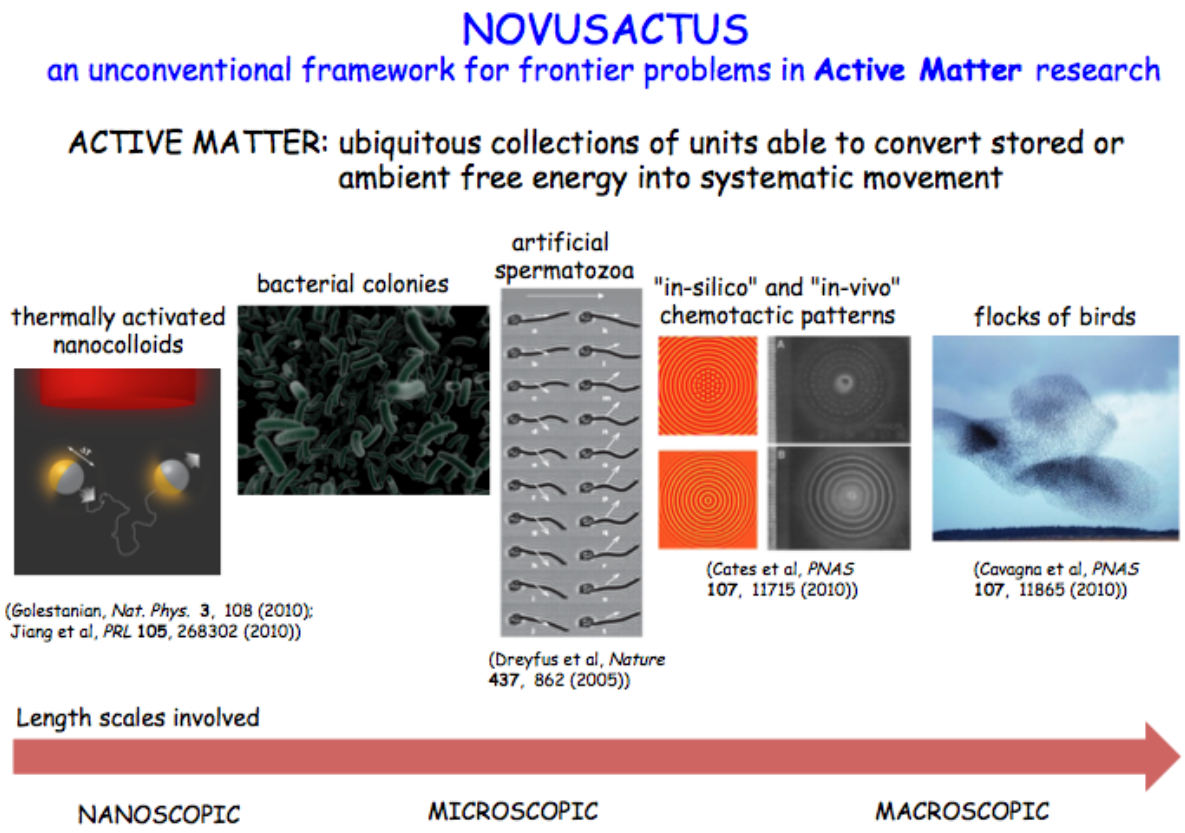
11 - Secondary ERC sub-sector
PE3_14 - Fluid dynamics (physics)

12 - Keywords

n°	Keyword
1.	NON-EQUILIBRIUM STATISTICAL MECHANICS
2.	SOFT MATTER PHYSICS
3.	BIOPHYSICS
4.	MICROFLUIDICS
5.	NUMERICAL SIMULATIONS

13 - Summary
Active Fluids are a fascinating example of Soft Matter, present everywhere in Nature, around us and inside us. Flocks of birds, swarms of microrobots, bacterial colonies, cell extracts of cytoskeletal filaments and motor proteins are instances of such systems. Active Fluids consist of collections of elements, embedded in a fluid environment, characterized by the common feature of being able to convert stored or ambient free energy into systematic movement, thus being intrinsically out-of-equilibrium. NOVUSACTUS will focus, in particular, on active particles of natural (**bacterial colonies**, algae, etc) or artificial (**active colloids**, microrobots) origin; these microswimmers can move by either mechanical means like rotating flagella, synchronized motion of cilia, body deformations or chemical processes, such as phoretic motion. Much theoretical effort has been spent, in recent years, in understanding the physics of locomotion of a single unit, while a clear picture of the implications of the mechanisms of swimming on the **collective dynamics** of suspensions of active particles is still lacking. Collections of microswimmers can display striking non-equilibrium phenomena: pattern formation, long-range correlations, flocking. The aim of NOVUSACTUS is to develop an **unconventional theoretical framework** and an **innovative multiscale numerical platform** to address fundamental and applied frontier questions on Active Fluids. The success of this high-risk project would unravel the basic mechanisms leading to collective phenomena and unusual rheological properties in wet active systems. Self-propelled objects in a community can interact and cooperate with each other either directly (e.g. by means of chemical signalling via pheromones) or through long range hydrodynamic perturbations induced in the suspending liquid by their motion. The absolute novelty of our methodology with respect to the state-of-the-art consists in that it will embrace mechanical locomotion and chemotaxis, quorum-sensing and resolved hydrodynamic interactions, integrating a particle-based description with a continuum approach.
Major theoretical and computational challenges in studying such problems come from the multiple scales and complex physics involved. This proposal has the unique feature of combining state-of-art numerical modelling (based on kinetic methods) with new phenomenological and theoretical ideas about the two-way coupling between continuum (hydrodynamical) and discrete degrees-of-freedom. Some key questions that I intend to answer are: How do microswimmers communicate? Which are the physical origins of their self-organization? Is it possible to control their aggregation to desing new *soft active materials*? What are their rheological properties? How do they react to imposed flow and confinement? What is the role played by solvent hydrodynamics? Is their any new physics behind the fluid

dynamics of an active suspension?
The proposed methodology stems from optimal numerical tools based on **Lattice Boltzmann Methods** (LBM). There are many advantages in using LBM to study flowing complex fluids in simple and complex geometries: i) the method is fully local in space, making upscale and parallelization effective; ii) it naturally describes a diffuse interface physics between different species and/or phases, without the need to track the interface; iii) it allows for simple and precise way to incorporate non-trivial fluid-solid interactions. The framework that I propose, with fully resolved hydrodynamics and self-propulsion mechanisms explicitely implemented, is absolutely innovative and promising to shed light on the importance of the key role played by the suspending liquid. The proposal will represent also a breakthrough among field-theoretical approaches, pioneering a continuum model of bacterial dynamics, including birth/death processes, coupled with hydrodynamics.



A.2 - INFORMATION ON THE HOST INSTITUTION

Host institution

Legal Name	Università degli Studi di ROMA "Tor Vergata"
City	ROMA (RM)
Address	Via O. Raimondo,18 Loc. La Romanina

Department/Faculty/Lab/Institute

Department/Faculty/Lab/Institute	Department of Physics
City	Rome
Address	Via della Ricerca Scientifica 1
Postal code	00133
Phone number	0672594300
E-mail address	fisica.dir@roma2.infn.it
Internet Home page	https://www.fisica.uniroma2.it/

1 - Brief analysis of the adequacy of the host institution to the goals of the proposal

The Statistical Mechanics group in the Department of Physics at the University of Rome “Tor Vergata” has a world-renowned expertise in the field of theoretical modelling and numerical simulation of fluid dynamics, from turbulence to microfluidics to complex fluids, using continuum and lattice-kinetic approaches. Recently, researchers in the group have been awarded with two ERC Grants: a 2011 Starting Grant (PE3 panel), DROEMU, "Droplets and Emulsions: Dynamics and Rheology" (PI: Mauro Sbragaglia), and a 2013 Advanced Grant (PE8 panel), NewTURB, "New eddy-simulation concepts and methodologies for frontier problems in turbulence" (PI: Luca Biferale). Sinergies between NOVUSACTUS and these two projects will lead to major breakthroughs. The expertise and tools developped/developping in the framework of DROEMU will certainly allow NOVUSACTUS to reach scientific results well beyond what could have been achieved in another host institution. Sinergies and overlaps will be exploited also with NewTURB, thanks to the activity in NOVUSACTUS meant to control the generation of motion by chiral-symmetry breaking active particles, which can preferentially inject helicity in complex flows, a crucial point for NewTURB. Thus, the host institution represents the perfect environment to develop the project; moreover, NOVUSACTUS will open a new line of research which will enrich the scientific landscape of the Department of Physics of Tor Vergata University with the establishment of a unique platform combining “in silico” and theoretical tools for multidisciplinary research in Active Matter.

A.3 - BUDGET

Budget

	O = Borne by other legal entities	H = Borne by the host institution	M = Borne by MIUR
A.1 - Staff of the host institution (professors, researchers, technicians, permanently employed; no to the fellows or graduate students, and so on, already under contract)		0	
A.2.1 - New contract for PI			145.176
A.2.2 - New contracts for researchers			244.080
A.2.3 - Fellows or similar already under contract	Not applicable	Not applicable	Not applicable
B - Overheads (60% A.1+A.2.1+A.2.2)			233.554
C - Equipment			50.000
D - Consulting services and similar			10.000
E - Other operating costs			27.000
F - costs borne by other legal entities	0		
G - Incentive for host institution			70.981
Partial costs	0	0	780.791

TOTAL COSTS: 0 € + 0 € + 780.791 € = 780.791 €

TOTAL FUNDING: 780.791 €

1 - Motivations of the expected costs

A: The project will cover full-time my research activity, whence the expenses for my salary for three years. Two PostDocs will be hired for 3 years each, to work on tasks T1 and T2 (see project description), at the 4th level: the requested salary is the maximum allowable such as to attract international top-ranked young scientists, able to work on cutting-edge problems.
B: Overheads will be used to organize two workshops and (partially) for travel expenses.
C: I intend to expand the local computing facility, consisting of two servers with four dual 6-core Xeon CPU, with 8 GB of RAM each, with 2 more servers configured as above, for a total estimated cost of about 50 Keuro.
D: International researchers will be invited for scientific collaborations on NOVUSACTUS topics, as stated in the project description.
E A lump sum of 3 Keuro per year has been allocated for each group member to travel and to attend conferences.

2 - Task carried out by other legal entities (item F)

3 - Permanent employees

Family name	First name	Institution	Department/Faculty/Lab/Institute	City	Country	Title (professor/researcher)

4 - Under contract personnel

Family name	First name	Department/Faculty/Lab/Institute	City	Country	Type of contract only on free funds of the host institution

5 - Personnel from other legal entity

Family name	First name	Institution	City	Country	Title (professor/researcher)

6 - Overall efforts in person-months

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B - RESEARCH PROPOSAL

B.1 - DETAILED DESCRIPTION OF THE PROJECT

1 - Objectives and expected results

A fascinating example of Soft Matter is provided by Active Fluids, i.e. collections of elements, embedded in a fluid environment, characterized by the common feature of being able to convert stored or ambient free energy into systematic movement, thus being intrinsically out-of-equilibrium. Instances of such fluids are cell extracts of mixtures of cytoskeletal filaments and motor proteins [1], which perform mechanical work at the expenses of the binding energy released in the ATP-hydrolisis, and suspensions of self-propelled particles of natural (bacterial colonies, sperm cells, algae, etc) or artificial (active colloids, microrobots [2]) origin; these microswimmers can move by either mechanical means like rotating flagella, synchronized motion of cilia, body deformations (most of bacteria, spermatozoa, algae) or chemical processes, such as phoretic motion induced by reactions (locally) catalyzed at the particle surface (active colloids) [3,4]. Due to their small sizes, microswimmers are subject to the physics of viscous hydrodynamics; as a result, in order to observe a net displacement, their movement must break the time-reversal symmetry [3,5]. Much effort has been spent in the understanding of the physics of locomotion of a single unit (see [3] and references therein), while a clear picture of the implications of the mechanisms of swimming on the collective dynamics of suspensions of active particles is still lacking [6,7]. Collections of microswimmers can display striking non-equilibrium phenomena, like pattern formation [8], long-range correlations and flocking [9,10]. The aim of this research proposal is to develop a new theoretical framework and to provide an innovative multiscale numerical platform to study active fluids. The realization of the project would unravel the basic mechanisms leading to collective phenomena in “wet” [7] active systems and enduing them with notable mechanical properties (complex rheology). Natural (bacteria, algae) and artificial (active colloids) self-propelled objects in a community can interact and cooperate with each other either directly (e.g. by means of chemical signalling via pheromones) or through long range hydrodynamic perturbations induced in the suspending liquid by their motion. The absolute novelty of our methodology with respect to the state-of-the-art consists in that it will embrace mechanical locomotion and chemotaxis, quorum-sensing and resolved hydrodynamic interactions, integrating a particle-based description with a continuum approach.

Major theoretical and computational challenges in studying such problems come from the multiple scales and complex physics involved: from the scale of molecules of solvent/chemicals (reactants/products for autocatalytic colloids, autoinducers for bacteria), to the microscale of swimmers, up to the macroscopic scale of aggregates, confining geometry and the active fluid as a whole. A certain coarse-graining is required. The proposed project has the unique feature of being of multiscale nature, thus allowing to adopt the proper focus, depending on the specific interest.

How do microswimmers communicate? Which are the physical origins of their capability to self-organize? Is it possible to control their aggregation to desing new “soft active materials”? What are their rheological properties? How do microswimmers react to imposed flow and confinement? What is the role played by the solvent hydrodynamics? Is their any new physics behind the fluid dynamics of an active suspension? These are the challenging questions I intend to answer in my project.

Depending on the presence or not of confining geometries and on the relevance of chemotactic couplings, the project can be divided in two main lines of research (with two sub-divisions each; see also figure 1).

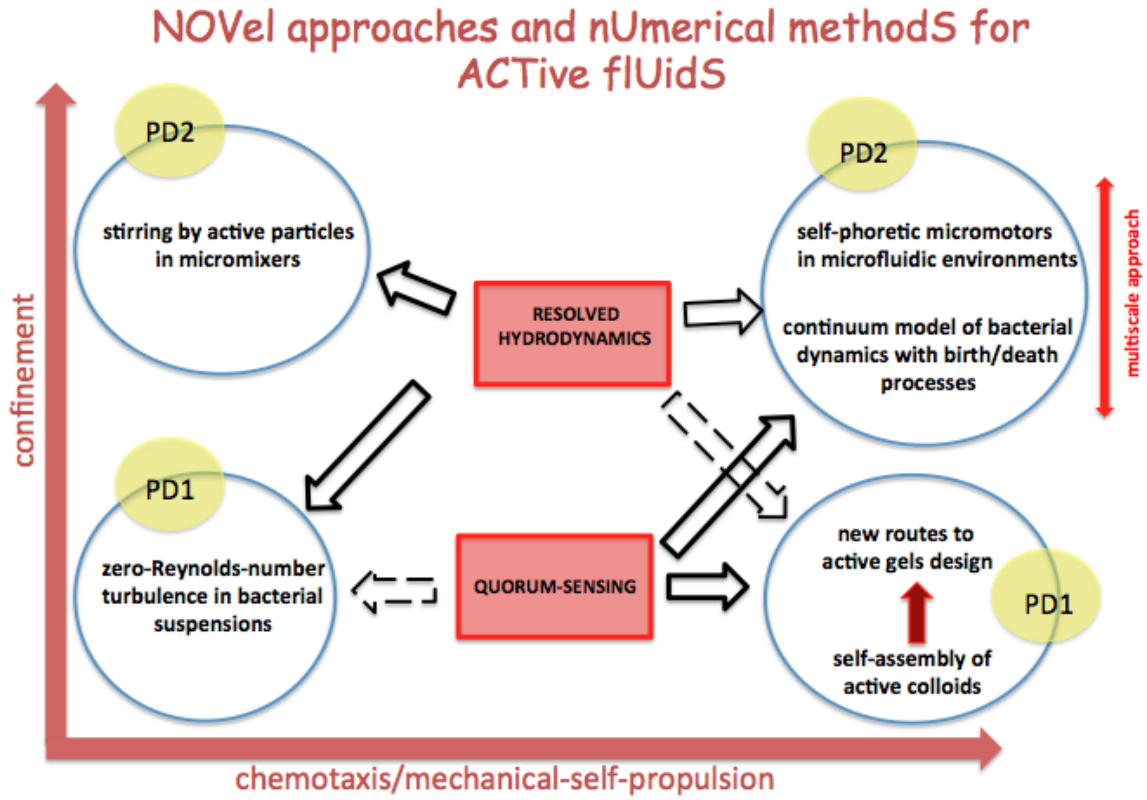
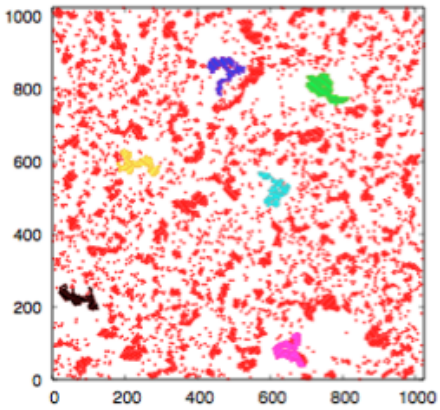


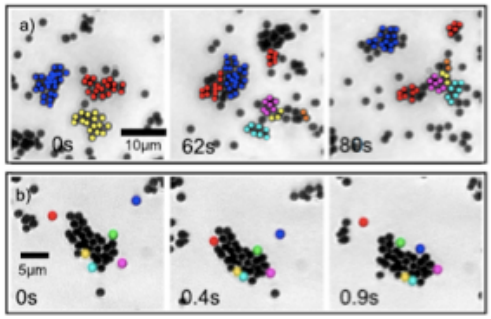
FIGURE 1: Summary of the project, highlighting two distinctive features of the research, fully resolved hydrodynamics and explicit quorum-sensing mechanism, and there relevance (encoded in the style of the arrows: dashed <-> less relevant, solid and thick <-> more relevant) in the various tasks, assigned to the two postdocs (PD1 & PD2).

COLLECTIVE DYNAMICS OF ACTIVE PARTICLES IN OPEN SYSTEMS. (T1)

The first task is to develop an innovative numerical model where microswimmers are treated as resolved finite size particles coupled with a coarse-grained description of the suspending fluid. An effective description of mechanisms like cilia motion or shape deformation, realized through prescribed boundary conditions at particles surfaces, will endow particles with the self-propulsion; on top of this, particles will produce and respond to a scalar field, whence being able to perform chemotaxis and self-phoretic motion and to develop collective chemical signalling (quorum-sensing). Such an unprecedented approach will enable to address the hydrodynamics of the active suspension from the bulk to the proximity of the particle, so that also near-field effects can be captured. In this way we may disentangle the two channels of communication, quorum-sensing and hydrodynamics, among self-propelling objects in order to clarify how they compete to the collective dynamics of the active system. According to the mechanism of self-propulsion, two main problems can be undertaken.
1) Self-assembly of active colloids. Depending on the type of affinity of the swimmer for the chemical field, different dynamic regimes can be imagined. For instance, if the interaction is attractive, we expect particles to self-assemble into aggregates (see figure 2) or percolating clusters, possibly leading to the discovery of a route to design novel active gels. To assess issues like the stability of the aggregates or the dynamical and rheological properties of active gels, large systems must be considered across large time scales, whence the need of exploiting high performance computing facilities.



LBM-based numerical simulations of self-phoretic colloids in 2d (A. Scagliarini & I. Pagonabarraga, to be submitted to PNAS)



Formation of clusters of self-phoretic colloids in the experiments of Theurkauff et al (PRL 108, 26833 (2012)); active particles here are microspheres of polystyrene coated with platinum, in a solution of hydrogen peroxide

FIGURE 2: Cluster formation observed in LBM simulations (left) and experiments (right) of self-phoretic colloids. Numerical simulations provide a unique flexibility in tuning the particle/chemical field affinity. If particles escape from high concentrations (chemorepellency), a completely different dynamic regime should be expected to emerge. We will explore the possibility of non-equilibrium phase transitions among these regimes at changing the model parameters.

2) Bacterial turbulence. For non-chemotactic swimmers, the only means of interactions is given by long range correlations due to viscous hydrodynamics. In this case, the particles movement, either coordinate or erratic, may induce a complex motion in the suspending liquid. Few recent studies have addressed the dynamics of the velocity field of the fluid, finding interesting features like anomalous diffusion of tracers and non-gaussian statistics [13]. Numerical simulations will allow us to undertake the first quantitative and systematic characterization of the statistical properties of the fluid velocity field (structure functions, energy spectra [14]) of a dilute active suspension, with the goal of revealing turbulent signatures at negligible Reynolds number (in analogy with studies of elastic turbulence [15]). Let us stress that, what I mean here is not the large scale structure formation or chaotic behaviour in collective bacterial dynamics at high concentrations [16], but the emergence of couplings across scales of fluid motion. Our focus differs, then, significantly, from that of recent works on ‘living turbulence' [17] in systems effectively equivalent to ‘dry' models [7].

ACTIVE SUSPENSIONS IN CONFINED GEOMETRIES UNDER FLOW. (T2)
The use of microdevices has become fundamental in experimental microbiology [12]; moreover, the dynamics of small sized swimmers in the proximity of liquid/solid interfaces is extremely relevant for processes such as biofilm formation and surface-crawling by microorganisms. This project provides a unique tool to study numerically confined active suspensions under imposed flow conditions, thanks to the versatility of the proposed methodology in handling complex geometries and suspended solid objects. These problems will be assessed at two levels of coarse-graining.
1) Finite size bacteria. The use of individual model bacteria (as described above) will allow to treat accurately hydrodynamics both in the bulk and close to particles surfaces (including, e.g., capillarity and lubrication effects). These studies may open the way to employ active particles to stir fluids in micromixers, a breakthrough for microfluidic research.
2) Continuum model of bacteria with birth/death processes and hydrodynamics. Taking into account birth and death processes in a colony is of crucial biological relevance in bacterial dynamics. Modelling such phenomena with a particle model would be unfeasible. Active fluids can be described by hydrodynamic equations for field variables representing, the density of particles, momentum and the orientational order parameter of the suspension (in analogy with the equations of liquid crystals but including “active” terms). For the first time in [11], bacterial population dynamics was described by means of a density field evolving according to a diffusion-reaction equation with an effective diffusivity depending on the local density istelf. The model proved to be able to reproduce non-equilibrium phase transitions, with formation of patterns strongly resemblant those observed in bacterial colonies.
The task, here, is to couple the continuum description of the bacterial density discussed above with the Navier-Stokes equation for the embedding fluid; the coupling will be implemented through the inclusion in the stress tensor of an active term, which we propose to derive (phenomenologically) from the bacterial density field.
The proposed theoretical scheme presents three absolute and fundamental novelties with respect to similar previous attempts: i) it does not require to consider also the equations for the vector orientational parameter, since the coupling between the active particles and fluid dynamics will be made directly with the density (or better with its gradients), and thus it appears to be suitable also to describe apolar particles; ii) it includes the “reaction” term standing for the birth/death processes of bacteria: notice that this term was crucial for the pattern formation observed in [11]; iii) the dynamics of the solvent is described explicitely.
The aimed development of this field model will allow us to carry out state-of-the-art numerical simulations to study the rheology of the active fluid and the effects of confinement and specific flows (e.g., shear or pressure driven) on the growth of bacterial population and on the stability of chemotactic patterns.

2 - State of the art

Although some of the considered systems (bacterial colonies) have been known and experimentally studied (with a biological focus) for years, the **physics of active fluids** can be considered a new and promising field of research. The state-of-the-art theoretical modelling of active systems is twofold [6,7]: in **agent-based models**, pioneered by Vicsek and coworkers [9], each active particle (at every time step) tends to align its (fixed magnitude) velocity vector with the average of its nearest neighbours, with noise acting against the alignment. Such models have proven to undergo a transition to a flocking state [9,16], at decreasing noise strength or increasing particle density; other models follow the same spirit but either at a kinetic [19] or "hydrodynamic" level [20], deriving **field equations** for averaged quantities (e.g. particle density and momentum) [6]. Continuum approaches for field variables based on equations analogous to those of liquid crystals (but including "active" terms) have been undertaken to focus on macroscopic aspects of active fluids, viz. large-scale instabilities and mechanical/rheological properties [7,21]. This project will go **beyond the outlined scenario** with the introduction of **new models** and **numerical schemes**. A **fully resolved** description of **hydrodynamics** and **self-propulsion** mechanisms makes it absolutely innovative and promising to shed light on the importance of the crucial role played by the suspending liquid. The proposal will represent also a breakthrough among field-theoretical approaches, pioneering a **continuum model of bacterial dynamics**, including **birth/death processes**, coupled with **hydrodynamics**.

3 - Methods

As pointed out in the objectives section, the kind of problems addressed in this project are intrinsically **multiscale**; therefore one should look for a **mesoscopic description**, which is provided by kinetic theory. The central quantity in this case, is the one particle probability density function, evolving according to the Boltzmann equation: **lattice Boltzmann Methods** (LBM) [22] are based on discrete versions of such equation (see figure 3) to simulate fluid systems at a coarser level (with respect to the atomistic one). These methods are **highly versatile**, thanks to the high flexibility in treating boundaries, introducing non-ideal behaviours (phase transitions), multicomponent mixtures and/or moving objects suspended in the fluid. Thus, LBM turn out to be extremely suitable to study complex systems such as i) multiphase fluids (complicated because of the presence of moving interfaces), ii) microfluidic systems, (where the fluid is typically confined in complex geometries at microscales, where the hydrodynamic limit breaks down and atomistic simulations can be computationally too expensive to simulate realistic time scales), iii) complex fluids, such as colloidal suspensions, gels, liquid crystals.
Furthermore, a crucial advantage of LBM with respect to all other numerical schemes stems from the fully local nature of interactions, allowing for **easy and effective parallelization and scalability** even in presence of complex boundary conditions. I have already available a **state-of-the-art 3d LBM** code for single- and multi-phase/multi-component fluids, with finite size resolved particles embedded. The code is fully MPI-parallel and portable on GPU based computers and showed excellent performance and scalability. These and several other features (temperature dynamics, fluctuating hydrodynamics, viscoelastic effects, modular implementation of geometry) make it a unique tool world-wide for complex fluids simulations. The code has been developed by researchers at the Universities of Rome and Eindhoven (including myself) and it is currently the reference numerical platform for research related to the ERC Starting Grant DROEMU.

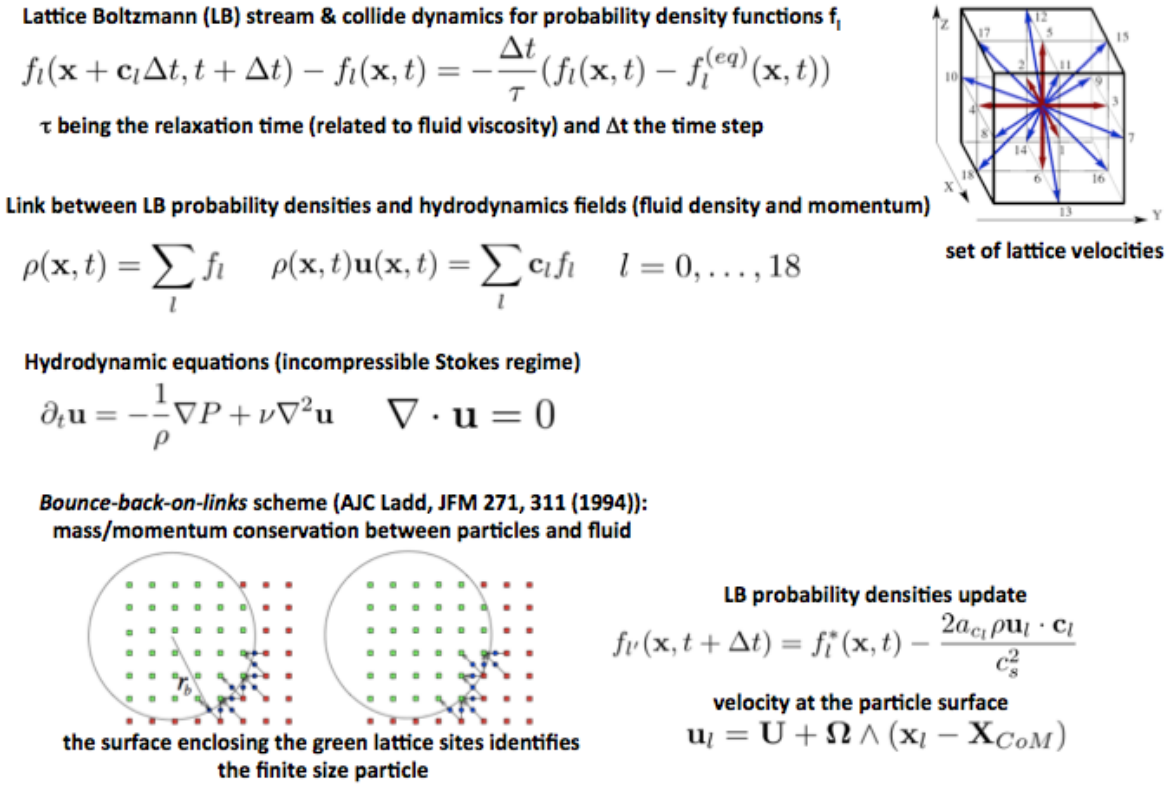


FIGURE 3: Lattice Boltzmann Method in a nutshell

ACTIVE PARTICLES. Finite size objects suspended in a solvent are described in the LB code as surfaces defined by a set of links between lattice nodes inside and outside. The correct momentum exchange between particle and fluid and the mass conservation through such boundary links are implemented according to Ladd's bounce-back-on-link scheme [23]. **Surface deformations** which induce bacteria self-propulsion will be mimicked imposing an **effective slip velocity**, variable over the particle surface. In this way, depending on the slip velocity profile, one can control both the swimming speed and the form of the velocity field generated by the swimmer. In particular, a version of the "squirmer" model [24] will be adopted. On top of this, we will implement the response of particles to a concentration field as well as a procedure for its production, in order to carry out the **first direct numerical simulation of autonomous motion and quorum-sensing-behaviour** following an **explicit mechanism**, as indicated by theoretical models of self-propulsion for autocatalytic colloids [25]. The use of active colloidal particles as artificial microscale swimmers is receiving an ever growing experimental interest [26], while the numerical counterpart is relatively poor. For instance, simulation studies of Janus particles (colloidal particles which are asymmetrically activated, e.g. coating only half surface with some catalytic agent, so to be able to self-propell in a proper environment) mainly involve the use of ad hoc devised phenomenological interaction potentials between an extra orientational degree of freedom of particles [27]. We will employ the described numerical scheme for 3d simulations in periodic systems to address the collective active colloids dynamics and self-assembly and the 'living turbulence' problem, as well as in complex geometries (from simple channels to straight ducts and T-/Y-junctions) and with imposed flows; up to billions of grid points with **millions of particles** will be needed, for a required computational effort of thousands of CPUs).

CONTINUUM MODEL. The aim is to develop a **new model** to couple the diffusion-drift equation equipped with a logistic-type growth term suggested in [11] for the bacterial density with Navier-Stokes hydrodynamics for the suspending fluid to perform the **first direct numerical study ever of bacterial dynamics** (including **birth/death processes** and chemotactic pattern formation) in **complex geometries** and under **flow**.

My proposal is to include an extra-term in the stress tensor appearing in the above mentioned equations, standing for the active contribution; such active stress will depend, through a constitutive relation, on the gradients of the density field.

A Gantt chart (figure 4) is provided summarizing the project schedule.

REFERENCES

[1] F. Julicher et al, *Phys. Rep.* **449**, 3 (2007).
[2] E.W.H. Jager et al, *Science* **288**, 2335 (2000).
[3] E. Lauga & T.R. Powers, *Rep. Prog. Phys.* **72**, 096601 (2009).
[4] W.F. Paxton et al, *J. Am. Chem. Soc.* **126**, 13424 (2004).
[5] E.M. Purcell, *Am. J. Phys.* **45**, 3 (1977).
[6] S. Ramaswamy, *Annu. Rev. Cond. Matt. Phys.* **1**, 323 (2010).
[7] M.C. Marchetti et al, *Rev. Mod. Phys.* **85**, 1143 (2013).
[8] E.O. Budrene & H.C. Berg, *Nature* **376**, 45 (1995).
[9] T. Vicsek et al, *Phys. Rev. Lett.* **75**, 1226 (1995).
[10] V. Schaller et al, *Nature* **467**, 73 (2010).
[11] M.E. Cates et al, *Proc.Natl. Acad. Sci.* **107**, 11715 (2010).
[12] A.K. Wessel et al, *Nature Rev. Microbiol.* **11**, 337 (2013); T. Ahmed et al, *Integr. Biol.* **2**, 604 (2010).
[13] K. Drescher et al, *Phys. Rev. Lett* **105**, 168101 (2010); J.S. Guasto et al, *Phys. Rev. Lett.* **105**, 168102 (2010).
[14] U. Frisch, Turbulence, Cambridge University Press (1995).
[15] A. Groisman & V. Steinberg, *Nature* **405**, 53 (2000).
[16] C. Dombrowski et al, *Phys. Rev. Lett.* **93**, 098103 (2004).
[17] H.H. Wensink et al, *Proc. Natl. Acad. Sci. USA* **109**, 14308 (2012); J. Dunker et al, *Phys. Rev. Lett.* **110**, 228102 (2013).
[18] G. Grégoire & H. Chaté, *Phys. Rev. Lett.* **92**, 025702 (2004); H. Chaté et al, *Phys. Rev. Lett.* **99**, 229601 (2007).
[19] D. Saintillan and M.J. Shelley, *Phys. Rev. Lett.* **100**, 178103 (2008).
[20] J. Toner & Y. Tu, *Phys. Rev. Lett.* **75**, 4326 (1995).
[21] A. Baskaran & M.C. Marchetti, *Proc. Natl. Acad. Sci. USA* **106**, 15567 (2009); R.A. Simha & S. Ramaswamy, *Phys. Rev. Lett.* **89**, 058101 (2002); Y.S. Hatwalne et al, *Phys. Rev. Lett.* **92**, 118101 (2004).
[22] C.K. Aidun & J.R. Clausen, *Annu. Rev. Fluid Mech.* **42**, 439 (2010); S. Chen & G. Doolen, *Annu. Rev. Fluid Mech.* **30** , 329 (1998).
[23] A.J.C. Ladd, *J. Fluid Mech.* **271**, 311 (1994).
[24] J.R. Blake, *J. Fluid Mech.* **46**, 199 (1971); T. Ishikawa et al, *J. Fluid Mech.* **568**, 119 (2006).
[25] R. Golestanian et al, *Phys. Rev. Lett.* **94**, 220801 (2007).
[26] J. Palacci et al, *Science* **339**, 936 (2013); J.R. Howse et al, *Phys. Rev. Lett.* **99**, 048102 (2007).
[27] F. Sciortino et al, *Phys. Rev. Lett.* **103**, 237801 (2009).
[28] K. Stratford et al, *Science* **309**, 2198 (2005).

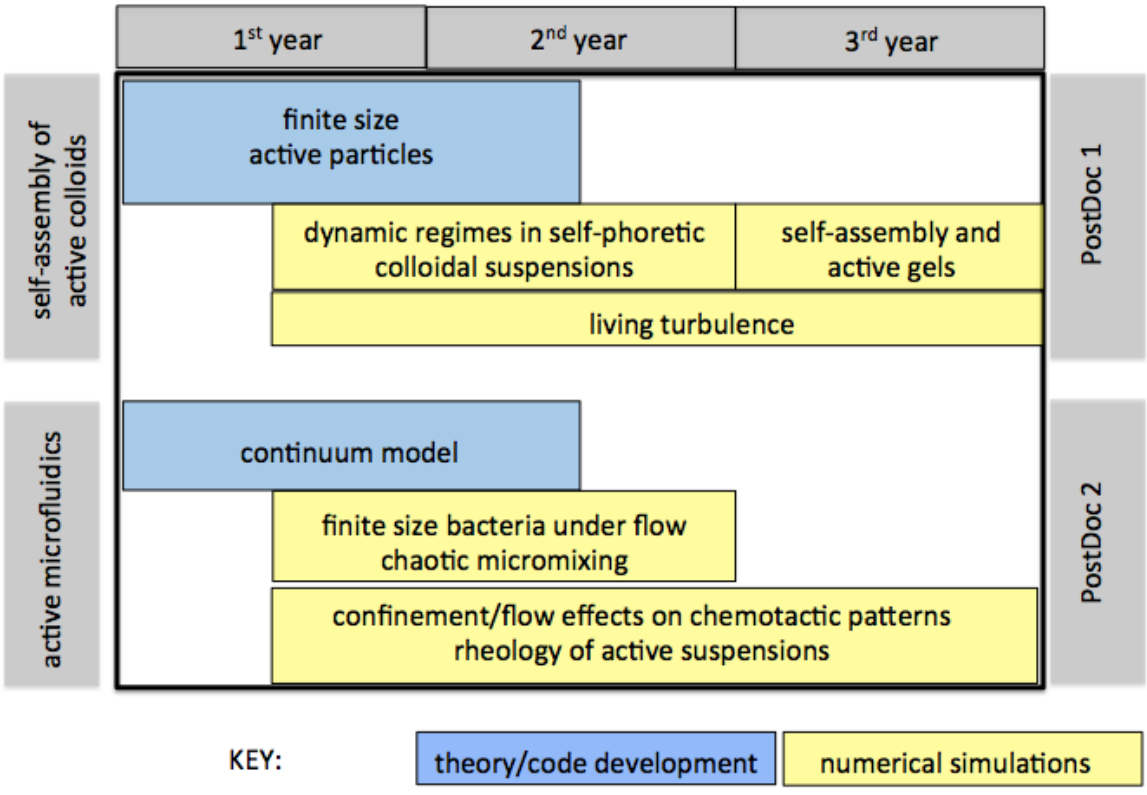


FIGURE 4: Gantt chart with a schematic project schedule

4 - Potential applications, scientific and/or socio-economic impact, technology advancements, brief remarks on ethical issues or security

Active fluids represent a challenging issue in non-equilibrium Statistical Physics and are also of utmost relevance in cutting-edge research field such as Biology and Nanotechnology. Tackling bacterial dynamics and microrobots design/control on the same footing, as envisaged by this research project, entails great scientific and cultural impact (think, e.g., to *swarm intelligence*). Shedding light on the fundamental mechanisms underlying the collective dynamics of microbial colonies, in fact, can be a key issue for the proper design of microrobots/active colloids; these, in turn, owing to their capability to generate autonomous motion at very small scales, may have potential applications to nanotechnological challenging situations such as the mixing of fluids confined in microfluidic devices (micromixers), or the controlled transport of material through nanopores. Moreover, some of the concepts and methods developed can be generalized to behavioural studies of other animal

communities, such as fish schools, insects hives, birds flocks.
From a macroscopic point of view, the study of these systems can be of relevance for Materials Science as well. Let us recall, indeed, that LBM-based simulations have anticipated experiments in the discovery of a new kind of material, the *bijel* [28], deriving from the different affinities between unmiscible liquids and suspended colloidal particles. In an analogous way, suspensions of artificial micro- and nanomotors may be expected to lead to the assembly of new active gels, with special mechanical properties. Concerning the bacterial turbulence problem, the capability of numerically designing microswimmers which generate controlled flows (for instance, injecting vorticity or helicity with a definite sign) at small scales and induce large scale motion due to collective effects, may have implications in the understanding of open issues in the theory of fluid turbulence.
NOVUSACTUS will enjoy collaborations with eminent international researchers. We will have interactions on model development and numerical implementation of self-propulsion for active colloids with Prof. I. Pagonabarraga (Barcelona) and with Prof. R. Golestanian (Oxford). Ideas on the continuum model of chemotactic bacteria with hydrodynamics will be exchanged with Prof. Pagonabarraga and with Prof. D. Marenduzzo (Edinburgh). We envisage also comparisons and integrative work with experiments on active microfluidics done in the group of Prof. F. Toschi (Eindhoven).
Finally, it must be remarked that no ethical or security issues apply for this project.

5 - financial aspects: expenditure estimates for each semester

	O = Borne by other legal entities	H = Borne by the host institution	M = Borne by MIUR
1st semester			171.799
2nd semester			121.799
3rd semester			121.799
4th semester			121.798
5th semester			121.798
6th semester			121.798
total	0	0	780.791

B.2 - CURRICULUM VITAE AND TRACK-RECORD OF THE PI

1 - Curriculum Vitae and track record of the PI

cv_scagliarini.pdf

C - SUPPORTING DOCUMENTATION

Scagliarini_dichiarazione_HI.pdf - Statement of the Host Institution concerning the conditions of autonomy of the PI
Ethics.pdf - Statement concerning the lack of impediments of an ethical nature
Security.pdf - Statement concerning the lack of impediments of a security nature

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