Consiglio di Amministrazione

Seduta del

18 MAR. 2014

Nell'anno **duemilaquattordici**, addì **18 marzo** alle ore **16.02**, presso il **Salone di rappresentanza**, si è riunito il Consiglio di Amministrazione, convocato con nota rettorale prot. n. 0016099 del 13.03.2014, per l'esame e la discussione degli argomenti iscritti al seguente ordine del giorno:

.... O M I S S I S ....

Sono presenti: il **rettore**, prof. Luigi Frati; il **prorettore**, prof. Antonello Biagini; i consiglieri: prof.ssa Antonella Polimeni, prof. Maurizio Barbieri, prof. Bartolomeo Azzaro, prof. Michel Gras, sig. Domenico Di Simone, dott.ssa Angelina Chiaranza, sig. Luca Lucchetti, sig.ra Federica Di Pietro; il **direttore generale**, Carlo Musto D'Amore, che assume le funzioni di segretario.

È assente giustificata: dott.ssa Francesca Pasinelli.

Assistono per il Collegio dei Revisori Conti: dott. Domenico Mastroianni, dott. Massimiliano Atelli (entra alle ore 18.25).

Il **presidente**, constatata l'esistenza del numero legale, dichiara l'adunanza validamente costituita e apre la seduta.

.... O M I S S I S ....

D.58/14
Personale
10.4

Consiglio di Amministrazione

Seduta del

18 MAR. 2014

SAPIENZA UNIVERSITÀ DI ROMA
Area Risorse Umane
Il Direttore
Dr.ssa Daniela Cavallo

SAPIENZA UNIVERSITÀ DI ROMA
Area Risorse Umane
Ufficio Personale Docente e Collaborazioni Esterne
Il Capo Ufficio
Dr.ssa Maurizia Valentini

FINANZIAMENTO DELLA COMUNITA' EUROPEA - GRANT AGREEMENT N. 339446 - PER L'ATTIVAZIONE DI UNA PROCEDURA DI RECLUTAMENTO DI UN RICERCATORE A TEMPO DETERMINATO TIPOLOGIA "A" PRESSO IL DIPARTIMENTO DI INGEGNERIA MECCANICA E AEROSPAZIALE

Il Presidente sottopone all'approvazione del Consiglio di Amministrazione la proposta del Dipartimento di Ingegneria Meccanica e Aerospaziale per l'attivazione di una procedura per il reclutamento di un Ricercatore a tempo determinato con regime di impegno a tempo pieno, per la durata di tre anni, eventualmente prorogabili per ulteriore due anni, tipologia A, per la realizzazione del programma di ricerca dal titolo a"Bubble nucleation on rough surfaces and cavitation inception", settore scientifico-disciplinare ING-IND/06 "Fluidodinamica" - settore concorsuale 09/A1 "Ingegneria Aeronautica, Aerospaziale e Navale". Il progetto è finanziato dalla Comunità Europea Grant Agreement n. 339446.

Ai sensi del decreto Legislativo n. 49/2012 ed in particolare dell'art. 5, commi 5 e 6, la proposta è stata inviata al Collegio dei Revisori dei Conti per il prescritto parere in ordine alla verifica della sussistenza di garanzie tese ad assicurare un finanziamento di importo e durata non inferiore a quella del contratto per il posto di ricercatore di cui all'art. 24, comma 3, lettera a) della legge 30 dicembre 2010, n. 240.

Il MIUR infatti, con nota del 5.04.2013 prot. n. 8312, ha posto come condizione all'autorizzazione nella procedura PROPER, dei contratti di ricercatore a tempo determinato, il rispetto delle suddette indicazioni.

In data 10 marzo 2014, il Collegio dei Revisori dei Conti ha reso parere positivo.

Alla luce di quanto su esposto il Presidente invita a deliberare.

ALLEGATI PARTE INTEGRANTE:

Progetto Grant Agreement n. 339446

ALLEGATI IN VISIONE:

Nota MIUR del 5.04.2013, prot. n. 8312;

Nota del 10.2.2014 del Dipartimento di Ingegneria Meccanica e Aerospaziale;

Verbale della seduta del 10.03.2014 del Collegio dei Revisori dei Conti.

SAPIENZA
UNIVERSITÀ DI ROMA

Consiglio di Amministrazione

Seduta del

18 MAR. 2014

.... O M I S S I S ....

DELIBERAZIONE N. 59/14

IL CONSIGLIO DI AMMINISTRAZIONE

- **Letta la relazione istruttoria;**
- **Visto lo Statuto dell'Università;**
- **Visto il Regolamento per il reclutamento di ricercatori con contratto a tempo determinato in vigore;**
- **Visto l'art. 24 della legge n. 240/2010;**
- **Visto il Decreto Legislativo n. 49/12, in particolare gli artt. 5 comma 5 e 7 comma 2;**
- **Vista la nota MIUR del 5.04.2013, prot. n. 8312;**
- **Visto il finanziamento della Comunità Europea – Grant Agreement n. 339446 al Dipartimento di Ingegneria Meccanica e Aerospaziale – D.I.M.A**
- **VISTO il verbale della seduta del 10.03.2014 del Collegio dei Revisori dei Conti;**
- **<u>Presenti 11, votanti n. 9</u>: con voto unanime espresso nelle forme di legge dal rettore e dai consiglieri: Polimeni, Barbieri, Azzaro, Gras, Di Simone, Chiaranza, Lucchetti e Di Pietro**

DELIBERA

di approvare il finanziamento della Comunità Europea ai fini dell'attivazione di una procedura di reclutamento di un Ricercatore a tempo determinato, tipologia A, con regime di impegno a tempo pieno per la durata di tre anni, eventualmente prorogabile per ulteriore due anni, settore scientifico-disciplinare ING-IND/06 "Fluidodinamica" - settore concorsuale 09/A1 presso il Dipartimento di Ingegneria Meccanica e Aerospaziale per lo svolgimento del programma di ricerca dal titolo: "Bubble nucleation on rough surfaces and cavitation inception"

Letto, approvato seduta stante per la sola parte dispositiva.

IL SEGRETARIO
Carlo Musto D'Amore

IL PRESIDENTE
Luigi Frati

.... O M I S S I S ....

10.4

SEVENTH FRAMEWORK PROGRAMME OF THE EUROPEAN UNION

EUROPEAN RESEARCH COUNCIL EXECUTIVE AGENCY

SP2-Ideas

Support for frontier research (ERC)

ERC Advanced Grant

ERC-2013-ADG

Grant Agreement Number 339446

BIC

Cavitation across scales: following Bubbles from Inception to Collapse

SEVENTH FRAMEWORK PROGRAMME

ERC GRANT AGREEMENT No 339446

PROJECT TITLE BIC

Support for frontier research (ERC)

ERC Advanced Grant

The **European Research Council Executive Agency** (the "*Agency*"), acting under powers delegated by the European Commission (the "*Commission*")

of the **one part,**

and UNIVERSITA DEGLI STUDI DI ROMA LA SAPIENZA, established in Piazzale Aldo Moro 5, ROMA, 00185, Italy represented by Giorgio Graziani, Director of Mechanical and Aerospace Engineering Department or his authorised representative, (the "*beneficiary*"),

of the **other part**

HAVE AGREED to the following terms and conditions including those in the following annexes, which form an integral part of this *grant agreement* (the "*grant agreement*").

Annex I - Description of Work
Annex II - ERC General Conditions - Single Beneficiary
Annex III - ERC accession forms for new and other *beneficiaries* to the *grant agreement.*
Annex IV - Financial statement form.
Annex V - a) 'Terms of reference for the certificate for the financial statements' and
b) 'Terms of reference for the certificate on the methodology'

Article 1 - Scope

The European Union ("*the Union*"), has decided to grant a financial contribution for the implementation of the *project* as specified in Annex I, called *Cavitation across scales: following Bubbles from Inception to Collapse* (*BIC*) (the "*project*") within the framework of the *SP2-Ideas* and under the conditions laid down in this *grant agreement.*

Article 2 - The *principal investigator*

1. The "*principal investigator*" as defined in Annex II is Prof. Carlo Massimo Casciola, born in Trevi (PG), Italy, on 10/01/1962.

2. The *beneficiary* shall enter into a *supplementary agreement* with the "*principal investigator*". The provisions of the *supplementary agreement*, which are not in accordance with this *grant agreement*, shall be deemed to be void for the purposes of this *grant agreement.*

3. Together with the signed *grant agreement* the *beneficiary* shall transmit to the *Agency* a signed copy of this *supplementary agreement.*

Article 3 - Duration and *start date* of the *project*

The duration of the *project* shall be 60 months from 1st February 2014 (hereinafter referred to as the "*start date*").

Article 4 - Reporting periods and language of reports

1. The *project* is divided into scientific reporting periods of the following duration:

- PA: from month 1 to month 30
- PB: from month 31 to the last month of the *project*.

Any scientific report required by this *grant agreement* shall be in English.

2. The *project* is divided into financial management reporting periods of the following duration:

- P1: from month 1 to month 18
- P2: from month 19 to month 36
- P3: from month 37 to month 54
- P4: from month 55 to the last month of the *project*.

Any financial management report required by this *grant agreement* shall be in English.

Article 5 - Maximum financial contribution of *the Union*

1. The maximum financial contribution of *the Union* to the *project* shall be EUR 2,491,200.00 (*two million four hundred and ninety one thousand two hundred EURO*). The actual financial contribution of *the Union* shall be calculated in accordance with the provisions of this *grant agreement*.

2. The financial contribution of *the Union* shall be in the form of a grant to the budget as specified in the table indicating the estimated breakdown of budget included in Annex I.

3. The bank account of the *beneficiary* to which all payments of the financial contribution of *the Union* shall be made is:

Name of account holder: DIPARTIMENTO DI INGEGNERIA MECCANICA E AEROSPAZIALE
Name of bank: UNICREDIT SpA - Roma 153
Account reference: IT17P0200805227000400014557

Article 6 - Pre-financing

1. A pre-financing of EUR 996,480.00 (*nine hundred and ninety six thousand four hundred and eighty EURO*) shall be paid to the *beneficiary* within 30 days following the date of entry into force of this *grant agreement*.

2. The *beneficiary* hereby agrees that the amount of EUR *124,560.00* (*one hundred and twenty four thousand five hundred and sixty EURO*), corresponding to the *beneficiary's* contribution to the Guarantee Fund referred to in Article II.20 and representing 5% of the maximum financial contribution of *the Union* referred to in Article 5.1, is transferred in their name by the *Agency* from the pre-financing into the Guarantee Fund. However, the *beneficiary* is deemed to have received the full pre-financing referred to in the first indent and will have to justify it in accordance with this *grant agreement*.

Article 7 - Special clauses

The following special clauses apply to this *grant agreement*:

Special clause 6

Notwithstanding the provisions of Article 6 the pre-financing shall be paid not earlier than 45 days before the *start date* of the *project*.

Special clause 39 ERC

In addition to Article II.30.3, the *beneficiary* shall deposit an electronic copy of the published version or the final manuscript accepted for publication of a scientific publication relating to *foreground* published before or after the final report in an institutional or subject-based repository at the moment of publication.

The *beneficiary* is required to make its best effort to ensure that this electronic copy becomes freely and electronically available to anyone through this repository:

- immediately if the scientific publication is published "open access", i.e. if an electronic version is also available free of charge via the publisher, or
- within 6 months of publication.

Special clause 40 ERC

1. In the case of transfer of the *grant agreement* to a new *beneficiary* upon request by the *principal investigator* and subject to approval by the *Agency*, the equipment items listed under the "equipment" budget category in Annex I and identified to be for the exclusive use of the project shall be transferred by the *beneficiary* to the new *beneficiary*

2. The new *beneficiary* shall reimburse the *beneficiary* for the remaining costs of the equipment which have not been depreciated. These costs as well as any accessory costs (for dismantling, transferring and installing the equipment) can be declared by the new *beneficiary* provided they fulfill the conditions stipulated in Article II.14 of the ERC *grant agreement* .

Article 8 - Communication

1. Any communication or request concerning the *grant agreement* shall identify the *grant agreement* number, the nature and details of the request or communication and be submitted to the following addresses:

For the *Agency*: European Commission
European Research Council Executive Agency
ERC Executive Agency - C2, COV2
Rue de la Loi 200
B-1049 Brussels, Belgium

For the *beneficiary*: Mrs. Giuseppina Angeloni
UNIVERSITA DEGLI STUDI DI ROMA LA SAPIENZA
Department of Mechanical and Aerospace Engineering
Via Eudossiana 18
Rome 00184
ITALY

2. Reports and deliverables shall be transmitted to the *Agency* according to Article II.4.6.

3. For information or documents to be transferred by e-mail, the following addresses shall be used:

For the *Agency*: ERC-C2@ec.europa.eu

For the *beneficiary*: giuseppina.angeloni@uniroma1.it

4. In case of refusal of the notification or absence of the recipient, the *beneficiary* is deemed to have been notified on the date of the latest delivery, if notification has been sent to one of the addresses mentioned in paragraphs 1 and 3 and to its legal representative.

5. Any communication or request relating to the processing of personal data (Article II.13) shall be submitted, using the address(es) for the *Agency* identified in paragraphs 1 and 3, to the controller responsible for the processing: Head of Department "Grant Management"

Article 9 - Applicable law and competent court

The financial contribution of *the Union* is a contribution from *the Union* research budget with the aim to implement the 7th Research Framework Programme (FP7) and it is incumbent on the *Agency* and the Commission to execute FP7. Accordingly, this *grant agreement* shall be governed by the terms of this *grant agreement*, the European Community and European Union acts related to FP7, the *Financial Regulation* applicable to the general budget of *the Union* and its *Rules of Application* and other European Community and European Union law and, on a subsidiary basis, by the law of Belgium.

Furthermore the *beneficiary* is aware and agrees that the *Commission* may take a decision to impose pecuniary obligations, which shall be enforceable in accordance with Article 299 of the Treaty on the Functioning of the European Union.

Notwithstanding the *Commission's* right to adopt directly recovery decisions referred to in the previous paragraph, the General Court, or on appeal, the Court of Justice of the European Union, shall have sole jurisdiction to hear any dispute between *the Union* and a *beneficiary* concerning the interpretation, application or validity of this *grant agreement* and the validity of the decision mentioned in the second paragraph.

Article 10 - Application of the *grant agreement* provisions

Any provision of this part of the *grant agreement*, shall take precedence over the provisions of the Annexes and the provisions of Annex II shall take precedence over the provisions of Annex I.

The special clauses set out in Article 7 shall take precedence over any other provisions of this *grant agreement*.

Article 11 - Entry into force of the *grant agreement*

This *grant agreement* shall enter into force after its signature by the *beneficiary* and the *Agency*, on the day of the last signature.

Done in two originals in English.

For the *beneficiary* done at ROMA

Università degli Studi di Roma La Sapienza
Name of the legal entity

Prof. Giorgio Graziani
Name of the legal representative

Stamp of the organisation (if applicable)

DIPARTIMENTO DI INGEGNERIA MECCANICA E AEROSPAZIALE SAPIENZA UNIVERSITÀ DI ROMA

Signature of legal representative

December 11th 2013
Date

For the *Agency* done at Brussels

Mechtild MAY
Head of Department

Name of the legal representative

Signature of legal representative

19 DEC 2013
Date

European Research Council

ERC Advanced Grant 2013
Research proposal [Part B1]

Principal Investigator: Carlo Massimo Casciola
Department of Mechanical and Aerospace Engineering
Sapienza University of Rome
via Eudossiana 18, 00184, Rome, Italy

Cavitation across scales: following Bubbles from Inception to Collapse

BIC

Project Duration: 60 months

Cavitation is the formation of vapor *cavities* inside a liquid due to low pressure. Cavitation is an ubiquitous and destructive phenomenon common to most engineering applications that deal with flowing water. At the same time, the extreme conditions realized in cavitation are increasingly exploited in medicine, chemistry, and biology. What makes cavitation unpredictable is its multiscale nature: nucleation of vapor bubbles heavily depends on micro- and nanoscale details; mesoscale phenomena, as bubble collapse, determine relevant macroscopic effects, e.g., cavitation damage. In addition, macroscopic flow conditions, such as turbulence, have a major impact on it.

The objective of the BIC project is to develop the lacking multiscale description of cavitation, by proposing new integrated numerical methods capable to perform quantitative predictions. The detailed and physically sound understanding of the multifaceted phenomena involved in cavitation (nucleation, bubble growth, transport, and collapse in turbulent flows) fostered by BIC project will result in new methods for designing fluid machinery, but also therapies in ultrasound medicine and chemical reactors. The BIC project builds upon the exceptionally broad experience of the PI and of his research group in numerical simulations of flows at different scales that include advanced atomistic simulations of nanoscale wetting phenomena, mesoscale models for multiphase flows, and particle-laden turbulent flows. The envisaged numerical methodologies (free-energy atomistic simulations, phase-field models, and Direct Numerical Simulation of bubble-laden flows) will be supported by targeted experimental activities, designed to validate models and characterize realistic conditions.

Section a: *Extended Synopsis of the project proposal*

Project presentation

The BIC (*Cavitation across scales: following Bubbles from Inception to Collapse*) project aims at establishing a new, integrated model for cavitation capable of describing its richness of scales, ranging from nucleation of bubbles to their transport and collapse. The success of the BIC project will supply on one side engineers with powerful predictive tools that could revolutionize the way of designing fluid machinery by accurately describing cavitation in macroscopic, typically turbulent, flows. On the other side, more recent applications of cavitation to medicine, chemistry, and material science will greatly benefit from the insight in micro and nanoscale phenomena promoted by the BIC project.

Cavitation has been an issue since the origin of hydraulic turbines and marine propellers, where it deteriorates and even destroys the blades and induces significant maintenance costs, see Fig. 1 and [1]. At a reduced scale it finds application in a variety of contexts like injection systems for liquid fueled engines, chemistry, and medicine. The essential notion of cavitation is that, when pressure is decreases below the saturation vapor pressure, vapor filled cavities (bubbles) may form in the liquid [1]. The nucleated bubbles grow and are transported by the flow. Pressure variations may also induce bubble collapse during which extreme conditions are realized leading, e.g., to cavitation damage on marine propellers. This simplified picture conceals the three main points that make cavitation so elusive:

1. **Cavitation inception mechanism:** liquids have a *tensile strength*, that is, they can withstand pressures well below the vapor pressure without cavitation to occur. The tensile strength highly depends on the liquid structure, on thermodynamic conditions, and, more importantly, on the presence of solid impurities and stabilized microbubbles that act as preferential sites for nucleation (*cavitation nuclei*) of vapor cavities. Cavitation inception, in short, is dictated by *microscopic* nucleation mechanisms.
2. **Nuclei and bubble transport:** along their trajectories, nuclei experience pressure variations that determine bubble growth, collapse, and rebound, see Fig. 1A. Knowledge of such trajectories is, therefore, crucial to predict where and how cavitation will occur. Turbulent conditions typical of engineering applications further complicate the problem leading to formation of clusters, vortex entrainment, and wall accumulation (*turbophoresis*).
3. **Bubble-flow interactions:** bubbles in flows are deformed by pressure gradients, coalesce, and break-up. The interaction between bubbles and the fluid environment are behind most of the macroscopic effects because of which cavitation is studied: cavitation damage, noise, sheet cavitation, sonoluminesce etc. For instance, the extreme conditions realized during anisotropic collapse of bubbles near solid walls cause catastrophic destruction of materials, see Fig. 1B.

In summary, in order to be *predictive*, models of cavitation cannot ignore its multiscale nature, that has its microscopic origin in nucleation, involves all the scales of turbulence, and leads to macroscopic

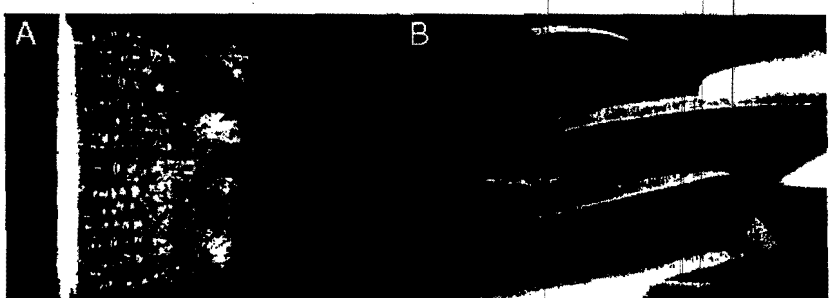

Figure 1. *A) Cavitation on a hydrofoil showing bubble nucleation and growth. B) Cavitation damage on pump blades (figures adapted from* [1]*)*

consequences of major importance.

Impact of the project on the state-of-the-art

Given its practical importance and the challenge for fundamental understanding, cavitation has been a long standing issue for a number of technical and scientific communities, including hydraulic engineering (Francis turbines, spillway tunnels of dams), mechanical, aerospace, and marine engineering (Diesel fuel injection systems, liquid oxygen turbo-pumps, ship propellers), chemical engineering (cavitation reactors), physics (fundamental understanding of nucleation, bubble chambers for high energy particle detection), chemistry (sonolumiscence and sonochemistry), and medicine (lithotripsy, sonoporation for drug delivery).

The engineering community developed a variety of models based on extensive experimental testing designed for specific applications, see e.g. [2] for marine engineering and [3] for fluid machinery. Such kind of approaches allowed significant advances in the related technologies, like e.g. the development of super-cavitating hydrofoils designed to prevent collapse of cavities on the surface of the body. However, in the aforementioned contexts, the use of computational fluid dynamics (CFD) as a design tool is hindered by the absence of predictive models accounting for nucleation, bubble transport, turbulence effect, bubble deformation and collapse. The main difficulty to overcome is that the microscopic nucleation process has a deep influence on cavitation inception and development, giving rise to a truly multiscale problem. As a consequence of the huge variety of applications where cavitation is crucial, very different *ad-hoc* approaches have been employed, while a comprehensive description of cavitation is still lacking.

From the fundamental point of view, the research focused on the nucleation processes and the related metastability of the liquid state [4]. Significant progresses have been achieved in homogeneous nucleation theory that correctly reproduces experimental data for pure liquids close to the critical point. However most engineering applications deal with water close to the triple point. In this case, even for purified water, the experimental data scatter becomes substantial suggesting that some form of *heterogeneous nucleation* is involved. It should also be stressed that in practice the working liquid contains most of the times a significant amount of solid impurities and surface-active molecules. This calls again into play the notion of heterogeneous nucleation [5,6], a subject which, despite of significant advances, still needs substantial improvement before reliable predictions could be made in engineering environments. An intermediate objective of the BIC project is to foster a new quantitative understanding of heterogeneous nucleation through new simulation techniques, that are sketched in the following. A more thorough understanding of heterogeneous nucleation will also prove instrumental to applications of *acoustic cavitation* in chemistry, material science [7], and medicine [8] where cavitation is induced by ultrasound forcing in a complex environment involving micro-particles as cavitation nuclei.

The main problem for establishing a comprehensive theory of cavitation is related to its intrinsic multiscale nature that embraces nano and microscales (nucleation), mesoscale aspects (bubble dynamics and deformation) and macroscale phenomena (interaction with flow, turbulence). **Objective of the BIC project is developing such a multiscale description of cavitation bridging the different scales involved in the process.** This objective is highly ambitious for the different kinds of expertise it involves and the intrinsic difficulty in matching phenomena occurring at such diverse scales; however its impact on the technical and scientific communities will be ground-breaking for the ubiquitous presence of cavitation in different technological and scientific contexts. In particular, the availability to the engineering community of predictive models and simulation techniques for cavitation, from nucleation to stress induced on solid boundaries, will lead to a **novel design of turbomachinery, marine propellers, hydraulic structures, and Diesel injection systems, and to the emerging medical and chemical technologies.**

Methodology

Along the years the PI of the BIC project explored many diverse aspects of fluid dynamics that include the effects of turbulence on combustion, particle transport, polymer additives, but also nanoscale wetting of superhydrophobic surfaces, capillarity, and protein translocation. For tackling such problems at the interface

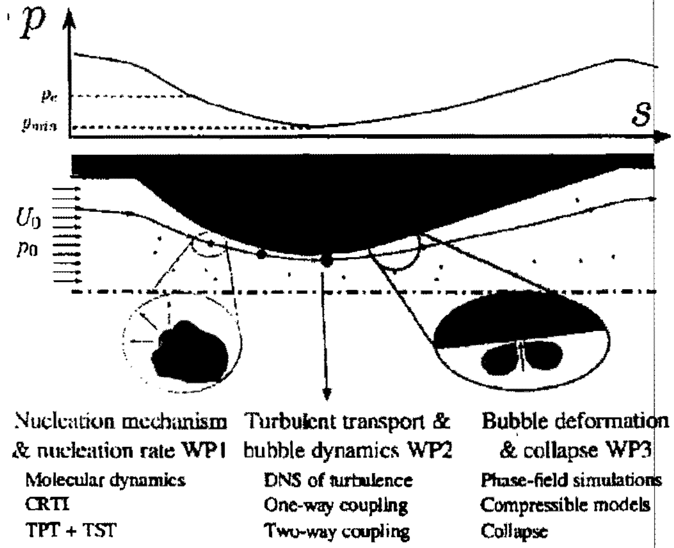

Figure 2: Sketch of a cavitating Venturi tube (center). *Solid impurities are transported by the flow, acting as cavitation nuclei. Following a nucleus trajectory, three events occur: 1) The pressure decreases below the cavitation limit* p_c *activating the nuclei which grow to form bubbles; 2) the bubbles are transported by and interact with the turbulent flow; 3) bubbles collapse at the Venturi wall where the pressure increases again. Pressure profile at the centerline is reported in top panel. The BIC project addresses each event by a dedicated Work-Package (WP), as outlined in the bottom panel and in the text.*

between engineering and mathematics, physics, chemistry, and biology many numerical techniques have been used and brought forward by the PI, including Direct Numerical Simulation (DNS) of particle-laden flows, phase-field models for multiphase flows, and advanced molecular dynamics techniques for nano-hydrodynamics (see Sec. *b* and *c* for further details and references). **The diverse skills acquired makes the proponent especially suited for tackling the multiscale description of cavitation, from the fundamental aspects of nucleation to the scales of typically turbulent flows encountered in engineeringapplications.** As anticipated the project concerns the development of a comprehensive model for cavitation, where all the scales of the phenomenology, from the nanometer scale of nucleation to the macroscopic scale of turbulence, are encompassed. Numerical simulations techniques capable of capturing the multiscale nature of cavitation will be developed and validated against targeted experiments. The unprecedented peculiarity of the proposed approach is its ability to properly couple the different stages of cavitation, from cavitation inception to bubble collapse in presence of solid boundaries typical of actual engineering configurations. A typical cavitating flow is illustrated in Fig. 2 to sketch the structure and objectives of the BIC project.

The BIC project is organized into four work-packages (WP), each developing a different aspect of cavitation, but closely interacting with the others. In the following we sketch the methodologies envisaged for each WP and the expected outcomes.

WP1: Nucleation mechanisms and nucleation rate

WP1 aims at providing theoretical and computational tools for accurately computing free energy barriers, nucleation mechanisms, and rates given the geometry and wetting properties of a nucleus as a function of thermodynamic conditions (pressure and temperature). Nuclei populations models will also be developed, with the support of WP4, in order to provide a viable input to the macroscopic flow description of WP2. In more details, this theoretical/numerical WP will take care of developing an advanced description of the micro and nanoscale mechanisms that are crucial in determining cavitation inception. Among these, probably heterogeneous nucleation in crevices [3] is the most important mechanism, for the ubiquitous presence of asperities in the bounding surface and, more importantly, in solid impurities advected by the flow. As sketched in Fig. 2, along their trajectories nuclei experience significant pressure variations (particularly in turbulent conditions) and may act as preferential sites for bubble nucleation and growth, dramatically influencing the cavitation inception limit. The heterogeneous nucleation problem will be dealt with atomistic and continuum methods coupled with advanced rare events techniques for estimating the bubble nucleation rate in the liquid, building upon the theory developed for rough hydrophobic surfaces in [PI1]. The approach implies the evaluation of the stability of nuclei and of the free-energy barriers that need to be overcome in the nucleation process of bubbles from single micro and nanoscale crevices as a function of the local liquid pressure. Various degrees of fidelity can be envisaged for the nucleation models, from the rough estimate provided by the restrained continuum model developed in our group [PI1] to the extremely sophisticated predictions based on restrained molecular dynamics [PI2] and on transition state theory [9]. Interaction with the experimental WP4 allows to both validate the models of nucleation and to characterize the geometry and chemistry of realistic nuclei. This WP is expected to bring about crucial step-wise advancements of the state-of-the-art of heterogeneous nucleation theories by the introduction of rigorous statistical-mechanics tools able to overcome the weaknesses of classical theories that are typically unable to predict the detailed form of the nucleation rate.

WP2: Turbulent transport and bubble dynamics

The main objective of WP2 is to describe the nuclei trajectories in turbulent flows, the early bubble dynamics activated by their pressure and temperature history, and the mutual interaction between flow and bubbles. In particular, the mutual coupling with the macroscopic flow simulation is necessary to obtain the trajectories of these putative cavitation nuclei. Once nucleation is successfully achieved, the micro-bubbles will be advected using a mixed Eulerian-Lagrangian algorithm like those successfully developed for particle transport in turbulence [PI3]. The micro-bubble descriptor will include the bubble characteristic dimension that obeys a Rayleigh-Plesset-like evolution equation [1]. This dimension changes in time due to the intrinsic dynamics of the bubble that is forced by the variation along the bubble trajectory of the external liquid pressure. It is well known [1] that during its evolution the bubble may exchange heat and mass with the surrounding. These effects call for considering the additional fields of temperature and concentration (e.g. the concentration field of dissolved gases) that influence the bubble dynamics in turn affecting the fields (*two-way coupling*). A crucial step in this part of the project will be developing new, fast, and accurate algorithms to allow such kind of two-way coupling. Indeed, given the potentially large number of transported bubbles, it is mandatory to overcome the limitations of the available techniques which typically work efficiently only for passive behavior of the transported phase (*one-way coupling*) [PI4], i.e. when the temperature and the concentration fields of dissolved species are not modified by diffusional exchanges with the interior of the bubble. A valuable by-product of WP2 will be the newly available ability of accurately describing momentum exchange between micro-bubbles and the liquid surroundings (e.g. for bubble-induced drag-reduction).

WP3: Bubble deformation, topological changes, and collapse

WP3 aims at describing the changes in topology of macroscopic bubbles due to shear stress, coalescence, entrainment in vortices, and non-spherical collapse via phase-field continuum models coupled with Navier-Stokes equations. Indeed, under the action of pressure gradients, bubbles grow to visible size and be significantly deformed; in addition, turbulence causes entrainment of bubbles in vortex cores and accumulation at walls [PI3]. In such conditions topology rearrangements are likely to occur, leading to merging of interacting bubbles. The so-called phase-field models will be employed to manage these complex phenomena. In these models, based on a properly defined free-energy functional, an evolution equation is devised for a suitable smooth scalar field (phase-field) that discriminates between liquid and vapor phase. A typical choice is the density of the fluid in the two (liquid-vapor) phases, which is assumed to vary smoothly between the two extrema corresponding to vapor and liquid. These models are able to account for surface tension and phase changes, e.g., via Van-der-Waals like equation of state with gradient penalization [10]. The phase-field couples to the Navier-Stokes equation via advection and (diffused) capillary stress at the interfaces [PI5], and is therefore compatible with the methods of WP2. These approaches are known to work effectively in simple geometrical settings. Here the challenge is the extension to complex geometries with the two-fold purpose of dealing with complex bodies (e.g. super-cavitating hydrofoils) and of addressing the heterogeneous nucleation on mesoscopic surface defects through the development of new immersed boundary techniques. This approach has been around for a while as concerning the single-phase Navier-Stokes (NS) equation [11]. Significant difficulties are known to emerge when the immersed boundary method is applied to the phase-field equation to be dealt with through innovative numerical formulations. An entirely new approach will be developed to allow the switching between newly nucleated, sub-grid, bubbles (described by the point-wise, Rayleigh-Plesset-like model of WP2) and mature, grid-resolved ones (tackled by the phase-field method). Another challenge of WP3 will be describing non-spherical bubble collapse at solid walls that is accompanied by liquid jetting and shock-waves at the origin of material damage [12]. A new compressible formulation of phase-field models and NS equations will be introduced in order to describe such extreme phenomena.

WP4: Experimental characterization and validation

This experimental WP is devoted to provide realistic inputs to the theoretical/numerical WPs through characterization of realistic conditions of cavitation and to validate the models developed along the BIC project. Relying on the facilities available at the Sapienza *Research Center for Nanotechnologies Applied to Engineering* (CNIS) micro and nanocharacterization and fabrication are already possible. In particular, Scanning Electron Microscopy (SEM) characterization of solid impurities as filtered from water will provide WP1 with realistic models for solid nuclei. Inspired by [13], experiments on cavitation inception will be pursued by measuring the nucleation pressure on crevices of controlled geometry realized by Focused Ion Beam (FIB) etching. These experiments will help validating the models of nucleation rates and mechanism developed by WP1. A new experimental setup will also be acquired for characterizing nuclei populations in water [14], that is a crucial step for bridging the description of nucleation (WP1) and the macroscopic transport and growth of bubbles (WP2). In the final phase of the project high-speed photography will be considered for imaging coalescence and collapse of bubbles, as a support to WP3.

Project outline

The final objective of BIC project will be achieved if WP1, WP2, and WP3 will not only produce innovative results in their own fields, but also supply an integrated description of cavitation. In order to achieve this objective, common milestones are envisaged, allowing to exchange ideas, intermediate results, and to bridge the different numerical techniques. On top of this organization scheme, the role of WP4 is designed to support this comprehensive view of cavitation, by feeding the other WPs with experimental data and insights.

The approach of the project will be chiefly theoretical and numerical, and for this reason around 65% of resources will be employed for hiring and forming new researchers with diverse backgrounds. However an important experimental section is also envisaged in order to support the project. For this reason approximately 20% of the project resources will be devoted to acquiring computational resources and new equipment, which will complement that already available at CNIS center. The remaining budget will be dedicated to disseminating the project results through peer-reviewed journals publications, participation to international conferences, workshops, and research visits to other institutions.

The BIC project will build upon the experience of the research group with multiple numerical techniques -more specifically rare events methods (WP1), particle-laden flows (WP2), phase-field models (WP3)- in order to promote a comprehensive understanding of a phenomenon, *cavitation*, that has an irreducibly microscopic origin and startling macroscopic consequences. In short BIC project would be the opportunity for a truly interdisciplinary and multifaceted scientific effort.

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Most relevant recent papers of PI on topics related to the BIC project

[PI1] A. Giacomello, M. Chinappi, S. Meloni, C.M. Casciola, *Metastable wetting on superhydrophobic surfaces: Continuum and atomistic views of the Cassie-Baxter/Wenzel transition.* Phys. Rev. Lett 109, 226102, 2012.
[PI2] A. Giacomello, S. Meloni, M. Chinappi, C.M. Casciola, *Cassie-Baxter and Wenzel States on a Nanostructured Surface: Phase Diagram, Metastabilities, and Transition Mechanism by Atomistic Free Energy Calculations.* Langmuir 28, 10764-10772, 2012
[PI3] F. Picano, G. Sardina, C.M. Casciola, *Spatial development of particle laden turbulent pipe flow*, Phys. Fluids, 21, 1-15, 2009.
[PI4] P. Gualtieri, F. Picano, G. Sardina, C.M. Casciola, *Clustering and turbulence modulation in particle laden shear flows*, J. Fluid Mech. 715, 134-162, 2013.
[PI5] F. Magaletti, F. Picano, M. Chinappi, L. Marino, C.M. Casciola, *The sharp interface limit of the Cahn-Hilliard/Navier-Stokes model for binary fluids*, J. Fluid Mech. 714, 95-126, 2013.

Section b: Curriculum vitae

Carlo Massimo Casciola leads a research group working on the fluid dynamics of complex flows based at the Mechanical and Aerospace Department of *Sapienza* University of Rome. The group consists of three permanent members among associate and assistant professors, and presently includes two postdocs and six PhD students. The *modus operandi* of the group is chiefly theoretical and numerical, oriented to fundamental and numerical modeling. This approach brought the group members to collaborate with scientists belonging to several neighbouring disciplines, such as physics, material science, chemistry, and biology. The issuing multidisciplinary and multiscale expertise has already proved successful in dealing with such diverse problems as Combustion, Drag reduction, Particle Transport, Multiphase Flows, and Interfacial Phenomena like wetting and liquid slippage. Major achievements of the research group under my guidance concern the coupling macroscopic flows with a micro-structure. In particular, the group has given contributions in particle-laden turbulent flows, polymer-laden and multiphase flows. Using Direct Numerical Simulation (DNS), significant insight has been provided for characterizing turbulent kinetic energy fluxes in wall bounded flows, where certain peculiar effects of reverse energy cascade associated with the *coherent vortical structures* were demonstrated to be fundamental for Large Eddy Simulations (LES) of wall bounded flows. More recently the interest enlarged to the nanoscale, and concentrated in the study of fluid motion and protein translocation in nanopores through various kind of Molecular Dynamics (MD) simulations. Finally advanced MD simulation and free-energy methods have been applied to address the stability of vapor nuclei on rough, hydrophobic surfaces. The original results achieved in this field encouraged us in extending this kind of approaches from the nano to the micro scale (thermodynamics and phase field methods).

Major research topics and contributions as senior author:

- *Particle-laden turbulent flows* (~20 papers among journals and conference proceedings; 2008-):
  Turbophoresis in wall flows (numerical, theoretical); Anomalous transport in cold jets (numerical, theoretical); Dynamics of inertial particles in reactive flows (numerical, experimental, theoretical); Clustering in homogeneous and inhomogeneous flows (numerical, theoretical)
- *Combustion* (~10 papers among journals and conference proceedings ; 2008-):
  Fractal behaviour of premixed flames (numerical, experimental, theoretical); Fractal-based LES modelling of premixed flames (numerical, theoretical); Counter-gradient diffusion in premixed flames (experimental, theoretical)
- *Micro-Nanofluidics* (~15 papers among journals and conferences; 2005-):
  Molecular Dynamics for fluid-flows through nano-pores (numerical, theoretical); Protein translocations through nano-pores (numerical, theoretical); Water slippage over hydro-phobic surfaces (numerical, experimental, technological)
- *Multiphase flows and phase change* (~ 6 papers among journals and conferences; 2010-):
  Phase-field methods (theoretical, numerical); Atomistic simulations and free-energy methods of wetting processes (theoretical, numerical)

Other research topics:

- *Visco-elastic turbulence* (~40 papers among journals and conferences; 1997-):
  Numerical modelling of drag-reducing polymer solutions (numerical, theoretical); Dynamics of long-chain polymers in turbulent fields (numerical, theoretical); Drag-reduction by polymeric additives (numerical; theoretical)
- *Scaling laws in turbulence* (~40 papers among journals and conferences; 1996-):
  Intermittency in shear dominated flows (numerical, experimental, theoretical); Scale-Energy fluxes in wall turbulence (numerical, experimental, theoretical); Universality in free turbulent jets (numerical, theoretical)
- *Aerodynamics* (~30 papers among journals and conferences; 1989-1998):
  Integral representation for vortical flows (theoretical, numerical); Aerodynamics of complex wing systems (theoretical, numerical)
- *Free-surface waves* (~10 papers among journals and conferences; 1989-1992):
  Numerical modelling and dynamics of non-linear water waves (theoretical, numerical)

Carlo Massimo Casciola, born 10 January 1962
Author Citation Profile: available on Google Scholar ; 734 citation, H-index 15. Number of international peer reviewed journal publications 61 (12 J. Fluid Mech., 12 Phys. Fluids, 3 Phys. Rev. Lett.).
Present position: Full Professor of Fluid Mechanics, Department of Mechanical and Aerospace Engineering, *Sapienza*, Italy
Previous Positions:

- Associate Professor at Dept. of Mechanics and Aeronautics, *Sapienza (*2000-2007)
- Research Assistant at Dept. of Mechanics and Aeronautics, *Sapienza (*1992-2000)
- Visiting professor of Gas-dynamics at Università degli Studi di Perugia (1990-1992)
- Researcher at INSEAN, Italian Ship Hydrodynamics Research Centre (1986-1992)

Appointments:

- Coordinator of the PhD Program in Theoretical and Applied Mechanics, *Sapienza (2007-)*
- Director of the Master Degree in Nanotechnology Engineering, *Sapienza (2008-)*
- Member of the EuroMech Turbulence Conference Steering Committee (2010-)
- Member of CNIS (Sapienza Industrial Nanotechnology Center) Directory Board
- Director of the CECAM Sapienza node (2012-)
- Editor of the journals Flow Turbulence & Combustion; Acta Mechanica; Meccanica

Funding ID:

- Sapienza Equipment Grant 2012: "*Shuttle and Find* Correlation Microscopy System for CNIS SEM and Fluorescence Microscope" (simultaneous acquisition at nano and microscale for bioapplications)

There is and there will be no funding overlap with the ERC Grant requested and any other source of funding for the same activities and costs that are foreseen in this project.
Completed projects:

- DEISA Extreme Computing Initiative (DECI-6) Grant winner *Particles in Boundary Layers* in collaboration with KTH Mechanics and TU/e Eindhoven (2010-2011).
- PRIN 2008 (2-years Research Projects of National Interest), *High Reynolds number wall-bound turbulence,* PI coordinating the activity of 4 different research units, Euro 150.000.
- PRIN 2005 (2-years Research Projects of National Interest), *Large scale structures in wall-bounded turbulence,* PI coordinating the activity of 4 different research units, Euro 130.000.
- Sapienza research program 2010 (1-year project): *Two-phase flows for propulsion,* PI, Euro 100.000.
- Sapienza research program 2007 (2-year project): *Turbulence transport, condensation and evaporation of droplet systems,* PI, Euro 80.000.

Research group outline: Fluid mechanics, Combustion and Micro/Nano Fluidics group at Sapienza Mechanical and Aerospace Eng. Dep.; 12 members among permanent staff, post-docs and PhD students and external associates.
International collaborations: I. Procaccia, V. L'vov (Weizmann Inst.); D. Henningson, E. Alfredsson, L. Brandt, P. Schlatter (KTH); B. Eckhardt (Philipps-Marburg Uni.); I. Marusic (Melbourne Uni.); E. Longmire (Minnesota Uni.); L. Bocquet (Lyon Uni.); K. Hanjalic (TU-Delft); I. Karlin (ETH); F. Toschi (TU Eindhoven); S. Meloni (UC Dublin).
Teaching:

- Micro/nano fluidics (Master Degree in Nanotechnology Engineering)
- Combustion and Turbulence (Master Degree in Mechanical Engineering)
- Vehicle Aerodynamics (Master Degree in Mechanical Engineering)
- Bio-fluid dynamics (Master Degree in Biotechnology)

Inspiring younger researchers:

- Supervisor of more 20 PhD students and more than100 graduate students.
- Among former (PhD or graduate) students:
    - 1 full professor in Sweden
    - 2 associate professors in Italy
    - 4 researchers in higher education institutions and research centres abroad

- about 10 Post-Docs in Italy and Europe (presently)
- about 10 PhD students in Italy and Europe (presently)

Achievements:

- Promoter and organizer of the Master Degree Nanotechnology Engineering at La Sapienza University, first initiative of this kind nationwide. The program started 2008 and is characterized by strong interdisciplinariety among different disciplines, Physics, Chemistry, Electronics and Mechanics and involves five different departments of Sapienza.
- Promoter of *Sapienza Industrial Nanotechnology Centre* and *Sapienza Nanoscience and Nanotechnology Lab.*

Section c: 10-year track-record

Bibliometry:

- 5-year author H-index (self-citations excluded): Scopus 8
- 10-year author overall H-index (self-citations excluded): Scopus 10
- H-index of 10 publications as senior author: Google Scholar 5, Scopus 4
- Total number of citations: Google 550, Scopus 362 (excluding self-citations)

10 publications of PI as senior author:

1. De Angelis, E., Casciola, C.M., Piva, R., *DNS of wall turbulence: dilute polymers and self-sustaining mechanisms.* Computers and Fluids, 31 (4), 495-507, 2002. *(Citations: Google Scholar 72, Scopus 54)*
2. De Angelis, E., Casciola, C.M., L'vov, V.S., Piva, R., Procaccia, I., *Drag reduction by polymers in turbulent channel flows: Energy redistribution between invariant empirical modes.* Physical Review E, 67 (5), 056312, 2003. *(Citations: Google Scholar 40, Scopus 31)*
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7. G. Troiani, M. Marrocco, S. Giammartini, C.M. Casciola, *Counter-gradient transport in the combustion of a premixed CH4/Air annular jet by combined PIV/OH-LIF.* Combustion and Flame, 156 3, 608-620, 2009. *(Citations: Google Scholar 9, Scopus 7)*
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10. A. Giacomello, A., Meloni, S., Chinappi, M., Casciola, C.M., *Cassie-Baxter and Wenzel States on a Nanostructured Surface: Phase Diagram, Metastabilities, and Transition Mechanism by Atomistic Free Energy Calculation,* Langmuir, 28 (29), 10764-10772, 2012. *(Citations: Google Scholar 1)*

Invited presentations and lecture series:

- Invited lecture series: Workshop/Autumn school on "Structures of the mechanics of complex bodies", C.M. Casciola, 4 lectures on *The structure of turbulence in Newtonian and viscoelastic flows: polymers and drag reduction,* Scuola Normale Superiore/Ennio De Giorgi Research Center for Mathematics , Pisa Italy, 2007.
- Invited tutorial: C.M. Casciola, *Scale-Energy Budget in Inhomogeneous Flow,* ETC11 Porto, Portugal, 2007.
- Cargèse Summer School on Anisotropic Turbulence: C.M. Casciola, 2 lectures on *Energy fluxes in*

anisotropic turbulence and *Particle clustering in turbulent jet flames*, Institut d'Etudes Scientifiques de Cargèse, Corsica, France, 2011.

- Short course: C.M. Casciola, *Advanced course on turbulent wall bounded flows*, Linné Flow Centre Graduate School KTH Mechanics, Royal Institute of Technology Stockholm, Sweden, 2008
- Short course: C.M. Casciola, *Numerical simulation of wall bounded turbulent flows*, Non equilibrium systems: Turbulence in fluids and plasmas, School in Matter Physics, Torino, Italy, 2004.

International conference organization:

- Member of the steering committee of the European Turbulence Conference (2010-)
- Organization of forthcoming ETC14 Conferences (Lyon 2013)
- Organizer of Turbulence, Heat and Mass Transfer (THMT) 12 (Palermo 2012).
- Organization of ETC13 Conferences (Warsaw 2011)
- Organizer of mini-symposium on *Multiphase Flows* at the AIMETA 2011 Conference
- Co-Organizer of AIMETA 2009 Conference, Ancona, Italy
- Co-Organizer of iTi Conference 2008 in Bertinoro, Italy

Awards:

- Sapienza Excellence Research Award 2010: *Turbulence in particle laden flows*

ERC Advanced Grant 2013

Part B2: *The Project proposal*

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

Project BIC takes up the long standing challenge of a providing a multiscale description of cavitation, from the nucleation to the collapse of developed bubbles. The variety of scales and phenomena involved requires a highly inter-disciplinary approach. Although the objective is an engineering one, the understanding of cavitation calls for a more fundamental knowledge of the physics and chemistry involved. **The key-point of the project is the development of robust and rigorous simulative tools to handle this multiplicity of scales and physics.** In the course of this endeavor, innovative tools will be developed, in three main fields, corresponding to three of the four work-packages (WP) that compose the project

1) Nucleation mechanisms and nucleation rate (WP1),
2) Turbulent transport and bubble dynamics (WP2),
3) Bubble deformation, topological changes, and collapse (WP3).

In the following, the state-of-the-art of these fields is reviewed to illustrate how the project will impact them. We also sketch the scientific background upon which the experimental section of the project (WP4) will build. The project is expected to push forward the state-of-the-art in all the three fields. However **the truly ground-breaking objective of the BIC project is incorporating all these innovations into a comprehensive multiscale description of cavitation.** This objective is both the most challenging and rewarding one, see Fig. 1.

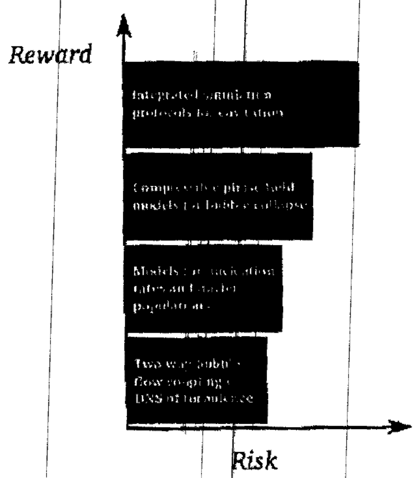


Figure 1: *Some of the most important objectives of BIC project, ordered in a hypothetical Risk-Reward scale.*

a1) Nucleation mechanisms and nucleation rate

It is always an arduous task to predict cavitation occurrence. This unpredictability is accentuated **for water near the critical point (the case of most engineering applications) where the cavitation pressure p_c is significantly above the homogeneous cavitation limit** [1], see Fig. 2. This limit is dictated by the competition of surface and volume free energies in the formation, in bulk liquid water, of spherical vapor cavities. In practical engineering situations, e.g. in designing marine propellers, either the cavitation pressure will be assumed to be the vapor pressure $p_c=p_v$ (an exceedingly conservative estimate) or it will be brutally underestimated by the homogeneous nucleation limit, see Fig. 2. Indeed, assuming homogeneous nucleation results in cavitation inception at pressures well above the design conditions, e.g., in a catastrophic overestimation of the limiting speed for cavitation (see inset *The cavitation number*).

To explain the departure from homogeneous nucleation theory, it is generally accepted that **bubbles preexist in any liquid as *cavitation nuclei*** [2]. The cavitation nuclei, as a catalyst, lower the free energy barrier necessary for a new bubble to nucleate, significantly increasing the cavitation pressure, see Fig. 2. Presence of dissolved gas in the liquid may further increase p_c. Nuclei survive to diffusion in the liquid because they are stabilized by a *skin* of surface-active molecules [3] (this model is called the *variable permeability model*), by trapping within *crevices* present on surfaces and small particles (the so-called *crevice model* [4]), or by a combination of the two mechanisms [5]. These theories are the only means, once some details about the nuclei are known, to predict the cavitation pressure (or, analogously, the cavitation inception number, see inset *The cavitation number*). For this reason, understanding the mechanisms of nuclei stabilization and predicting their evolution is becoming more and more important for engineering, in view of improved design aided by CFD, e.g., in marine and hydraulics applications [6].

The limitations of the current nucleation theories, in particular the *crevice* model, are due to **strong metastabilities encountered in bubble nucleation from rough surfaces** (it is actually a *rare event* as demonstrated in [7] for the wetting of superhydrophobic surfaces). Sophisticate simulation techniques are needed to cope with such metastabilities in order to predict effective nucleation mechanisms and rates. In this direction, **we recently proposed simulation methods based on free energy molecular dynamics (MD) techniques [7] and on a novel continuum restrained thermodynamic integration (CRTI) method [8] that could prove breakthrough-tools in developing rigorous theories for cavitation nuclei,** see Sec. *b*.

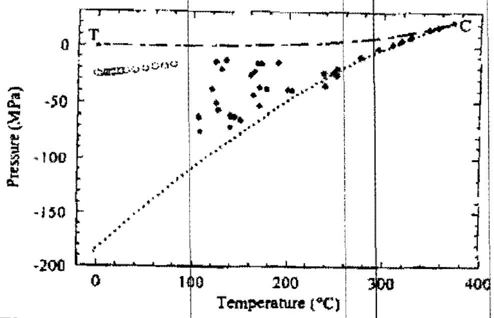


Figure 2: Experimental cavitation pressure p_c *(symbols), homogeneous nucleation theory (dotted line), and liquid-vapor coexistence pressure (dash-dotted line) for pure water. Triple and critical points are indicated as T and C, respectively. Adapted from* [1].

The cavitation number

In many situations the order of magnitude of the pressure minima occurring in the flow can be roughly estimated before hand. This typically happens for external flows, such as the flow over an immersed body like a hydrofoil. In this case, outside the boundary layer close to the body surface, the classical Bernoulli equation from elementary fluid mechanics provides a link between flow velocity and pressure

$$p+\frac{1}{2}\rho_f u^2=p_0+\frac{1}{2}\rho_f U_0^2 \quad ,$$

where the subscript zero denotes free stream conditions away from the body. The pressure coefficient provides a dimensionless form of the pressure difference with the free-stream,

$$C_p=2\frac{(p-p_0)}{(\rho_f u_0^2)} \quad .$$

For external flows with thin attached boundary layers the C_p distribution on the body surface is controlled by the body geometry (potential aerodynamics). More specifically, when the external stream is irrotational, the velocity u is the gradient of the scalar potential solution of the Laplace equation $\nabla^2\phi=0$. In this conditions classical theorems on elliptic partial differential equations state that pressure extrema (in particular the minimum value of pressure coefficient, here indicated as C_{pmin}) are achieved at the boundary of the domain, implying that cavitation inception and bubble collapse are expected to occur right at the solid boundary. The cavitation number $\sigma=2(p_0-p_v)/(\rho_f U_0^2)$,

estimates "how far" cavitation is from the free-stream conditions. When $C_{pmin}=-\sigma$, it is expected that cavitation inception happens right at the pressure minimum. From this condition is possible to obtain an estimation of the critical free stream speed above which cavitation is expected to occur. However nucleation theory shows that this condition is almost always inappropriate, since the actual flow is seeded with cavitation nuclei. Actually, typically cavitation occurs at much larger pressures than expected on the sole basis of the equilibrium vapour pressure of the pure liquid, see Figure 2.

a2) Turbulent transport and bubble dynamics

The nuclei advected with the flow experience pressure variations enhanced by the turbulence, which is present in most engineering applications. These variations cause the nuclei to grow into bubbles of visible size, to collapse, and rebound [9]. Whereas in the early phase of growth the bubbles may be considered spherical, anisotropies in the flow (due, e.g., to solid walls) cause the bubbles to deform. For instance, the complex mechanism of cavitation damage may be ascribed to the dramatic effects of collapse of non-spherical bubble on walls [10], see the next paragraph on WP3 background. In the context of WP2, we review the state-of-the-art of simulations of bubble-laden flows in the early stage of growth from nuclei, when the bubble dynamics obeys a version of the Rayleigh-Plesset (R-P) equation [11], see inset *The*

The Rayleigh-Plesset equation

The Rayleigh-Plesset equation,

$$R\ddot{R}+\frac{3}{2}(\dot{R})^2=\frac{1}{\rho}(p_i-p_\infty-2\frac{\sigma}{R}-4\mu\frac{\dot{R}}{R}) \ ,$$

describes the evolution of the radius of a spherical bubble immersed in a liquid. It rules the evolution for the bubble radius R and it is obtained by integrating the Navier-Stokes equations for the liquid motion outside the bubble resulting from the (still unknown) variation of the bubble radius. The driving force is the difference between the pressure far away from the bubble and the pressure at the liquid/bubble interface. The latter depends on the pressure p_i inside the bubble and on the surface tension σ at the liquid-vapour interface, via the bubble curvature radius R. When the external pressure p_∞ changes with respect to the equilibrium condition stated by the Young-Laplace equation, $p_\infty^{eq}-p_i=-2\sigma/R$,the bubble radius is forced to change, expanding or contracting depending on the sign of the actual pressure difference $p_\infty-p_\infty^{eq}$. The liquid viscosity tends to dump the consequent motion. The bubble dynamics is strongly influenced by inertial effects which are responsible for the strongly non-linear character of the equation implied by the quadratic term in the time derivative of the bubble radius. The phenomenological consequences of this non-linearity is the existence of a critical radius R_c above which the bubble becomes unstable. Depending on external conditions the bubble either expands (cavitation reaching visually detectable levels) or explosively contracts (bubble collapse).

Rayleigh-Plesset equation. This equation describes the oscillations of spherical bubbles, and, since the pioneering work of Johnson and Hsieh [12], has been coupled to the Navier-Stokes equations to investigate the influence of nuclei trajectories on cavitation inception (see also [13] for an Eulerian formulation with prescribed number density of bubbles). Turbulence has been addressed in this context by coupling the Lagrangian description for the bubble trajectories with the so-called Reynolds Averaged Navier-Stokes (RANS) [14]. Alternative to Lagrangian approaches, RANS solvers have also been coupled with the vapor mixture fraction equation solved on an Eulerian grid, see e.g. [15] where this formulation is combined with the Rayleigh equation for vapor mass production/destruction. All these empirical approaches are based on several flow-dependent assumptions and tuning coefficients.

In order to overcome the apparent limitations of the available approaches, a description of the cavitating flows is here envisaged where Direct Numerical Simulation (DNS), able to reproduce the detailed turbulent dynamics, is coupled with the Lagrangian description of the bubbles, along the line of [16]. This approach has been already applied by our group in flows laden with solid particles [17] and extended in [18] to include the back-reaction of the transported phase on the carrier fluid. The Lagrangian description of small bubbles relies on the idea that a small immersed object perceives a substantially uniform flow velocity when it is smaller than the relevant length scale of velocity variation. In a turbulent flow such minimal length is the the so-called Kolmogorov scale [19]. Hence sub-Kolmogorov bubbles are subject to the fluid forcing described in [16], see the inset *The Maxey-Riley Equation*. The bubble responds to the pressure in the fluid, an effect of paramount importance in turbulence, where coherent vortical structures with low pressure cores of different scales dominate the dynamics. **Bubble are strongly sensitive to this peculiar pressure distribution** since: i) the pressure reduction inside the vortex cores may activate new cavitation nuclei while making the existing bubble grow; ii) the bubbles are forced towards the low pressure regions by the pressure gradients increasing the probability of bubble merging. Without discussing here bubble topological changes, treated in the next section, it worths stressing that a strong coupling exists between turbulent flow, Maxey-Riley dynamics, and the Rayleigh-Plesset evolution for the bubble radius. The scenario becomes even more entangled when the bubbles modify the liquid environment, as it happens when:

a) **The bubble volume fraction increases enough to make the momentum exchange between cavitation bubbles and liquid able to alter the liquid dynamics.**

b) **The bubble dynamics couples to thermo-kinetic effects** such as heat transfer with the liquid fostered by temperature changes due to, e.g., compression work on the bubbles and latent heat.

The bubble population has in general active effects on the liquid in the two-way coupling regime (as opposed to the one-way coupling regime where the liquid is unperturbed). Due to the back-reaction associated with the Stokes drag, the fluid velocity is altered by the bubble, changing the nearby convection velocity. **Such**

fluid-mediated interactions are important for bubble swarms, specifically for bubble coalescence. All these crucial effects are beyond the reach of present state of the art simulations. The new cutting-edge description of bubble-flow interactions of the BIC project is expected to shed new light on nuclei transport, bubble growth, bubble clustering and their eventual collapse in turbulent flows.

a3) Bubble deformation, topological changes, and collapse

After bubbles grow to sufficiently large size, flow anisotropy induces significant deformations, and eventually the bubble can break-up into smaller fragments. The opposite event is also frequently observed as merging of bubbles occurs, due to bubble-bubble collisions [20]. These effects are clearly expected for large bubbles, but also small bubbles may merge due to added mass effects (see inset *The Maxey-Riley equation*) that cause preferential concentration (clustering) [21] inside vortex cores. Flow inhomogeneities due to solid walls also contribute to strong bubble segregation via turbophoresis (transport induced by turbulence inhomogeneity, see [22], [23] for the related case of solid particles and [24] for bubbles). Hence, spatial segregation and clustering concur in increasing the coalescence probability. **All these effects call for innovative approaches able to tackle extreme deformations and topological changes of the bubbles while resolving the turbulent dynamics.**

When the bubble enters a region of pressure exceeding the equilibrium pressure, it starts shrinking to eventually collapse. This is an inertia-dominated process: once started, liquid converges towards the shrinking bubble and a catastrophic chain of events is originated. Although the spherically symmetric problem may be treated with the Rayleigh-Plesset equation, the actual collapse phase is more complicated [11; 25] since during sudden shrinking the spherical shape is easily destabilized. Any external influence that breaks the radial symmetry of the liquid inrush ends up with strong anisotropy of the collapsing bubble. In practice the most relevant case is a solid wall that promotes symmetry breaking of the bubble collapse.

Anisotropic collapse has been extensively treated in the literature [10; 26-28]. The numerical solution of the simplest model problem [29], based on the irrotational flow assumption, confirms the experimental finding [30] that bubble collapse near solid walls is associated with intense micro-jets impinging the wall.

The Maxey-Riley equation

The equation derived by Maxey and Riley [16],

$$m_c \frac{d v_p}{dt} = \frac{3}{2} m_f \frac{D u}{Dt} - 6\pi R \mu (v_p - u) - 6\pi R^2 \mu \int_0^t \frac{d/d\tau (v_p - u)}{\sqrt{\pi \mu/\rho (t-\tau)}^{1/2}} d\tau + O(R^2) \quad ,$$

describes the advection of a small spherical particle with velocity $v_p(t)$ by the liquid velocity field $u(x,t)$. The particle is assumed to be much smaller of the scale over which significant spatial variation of liquid velocity occur. Corrections associated to the liquid velocity non-uniformity are not shown explicitly and are clumped in the last term where they are indicated as second order correction terms. The effective mass of the particle is $m_e = m_p + 1/2\, m_f$ where m_f is the mass of fluid that would correspond to the particle volume. The effective bubble mass is increased by the so-called *added mass* of the liquid. In the case of a vapour bubble its intrinsic mass is negligible and the effective mass equals the added mass, i.e. half the mass the particle would have, were it liquid instead of gaseous. The first term on the right-hand side is proportional to the fluid acceleration and describes the migration of the bubble under a pressure gradient in the liquid, as follows from the Euler equations of motion for the liquid that are reported here instead of the full Navier-Stokes equations for the sake of conciseness,

$$\rho_f \frac{D u}{Dt} = -\nabla p \quad .$$

The second term on the right-hand side is the Stokes drag, describing the viscous resistance the particle experiences in the relative motion with the surrounding liquid. Due to this viscous interaction the bubble is dragged along with the liquid flow. The bubble accommodates the liquid velocity variation with a relaxation time $\tau_p = m_e / 6\pi R \mu$, expressed in dimensionless form as the Stokes number $St = \tau_p / \tau_f$, ratio of bubble relaxation time to a characteristic fluid dynamics scale. The third term may also be important for cavitation. This Basset force accounts for a memory effect induced on particle motion by the vorticity that the particle sheds in its wake. Although the relative motion between bubble and liquid is small, so that the wake is weak, this term may have significant influence.

Level-set method and hyperbolic solvers

The level-set method is a computational technique used to advect spatial domains with the flow velocity $\boldsymbol{u}$. In the present case the relevant domain is the gas bubble B , and its indicator function

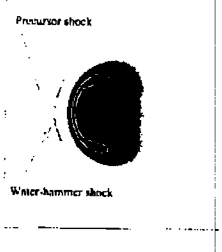
$$\phi(\boldsymbol{x},t)=\begin{cases} 1\, if\, \boldsymbol{x}\in B \\ 0\, if\, \boldsymbol{x}\notin B \end{cases}$$

evolves according to the transport equation

$$\frac{\partial \phi}{\partial t}+\boldsymbol{u}\cdot\nabla\phi=0 \ .$$

The numerical tools used to solve the equation are taken from the machinery of solvers for hyperbolic equations based on shock-capturing schemes (as opposed to the more traditional shock fitting methods), able to track the discontinuities (either contact or shock discontinuities) of solutions of hyperbolic systems of conservation laws. The interest is here on the compressible Euler system,

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\boldsymbol{u})=0$$
$$\frac{\partial(\rho\boldsymbol{u})}{\partial t}+\nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u}+p I)=0$$
$$\frac{\partial(\rho e)}{\partial t}+\nabla\cdot[\rho\boldsymbol{u}(e+p)]=0$$
$$\frac{\partial[\rho f(\phi)]}{\partial t}+\nabla\cdot[\rho\boldsymbol{u} f(\phi)]=0$$



involving fluid density, velocity and internal energy, respectively. In the last equation $f(\phi)$ is any function that takes two different constant values inside and outside the bubble, respectively. Under the assumption of negligible viscosity and surface tension the evolution of a gas-filled bubble has been recently simulated by numerically solving the above system [28], see the figure. The system is completed with a suitable equation of state, $p+kA=(k-1)\rho(e-1/2\boldsymbol{u}\cdot\boldsymbol{u})$ with $k(\phi)$ and $A(\phi)$ such that the perfect gas and a Tait-like equation of state for (compressible) liquid water are recovered inside and outside the bubble, respectively. In Eulerian based computational methods the solution is smoothed over a few grid nodes. Suitable schemes, e.g., essentially non-oscillatory (ENO) or weighted essentially non oscillatory (WENO) schemes are used to discretise the system on the grid. Without entering here into the numerical details, see e.g. [33], in view of the BIC project it is worth stressing that such an approach, though capable of dealing with extreme bubble deformations and related shock dynamics, can hardly cope with topological changes of the bubble.

The associated water-hammer is believed to be one of the reasons for the fast degradation of material exposed to cavitating flows. Another explanation is the propagation of shock-waves in the liquid [31]. Recent simulations [28] with an inviscid compressible model (Euler equations) where the bubble interface is described by the so-called level-set method [32] (see also the inset *Level-set method and hyperbolic solvers*) have succeeded in capturing the shock waves, the formation of the micro-jet and their interaction with the wall. This simulation, although relying on significant simplifying assumptions (negligible surface tension and viscosity, gas filled cavity), is extremely interesting in showing the clusive sequence of events occurring when bubbles collapse near a wall.

Concluding this brief survey on bubble deformations, coalescence, break-up, and collapse, it is worth stressing that **a general approach able to encompass all these aspects and couple them with a background turbulent flow is still lacking**, while *ad hoc* solutions have shown their importance in cavitation phenomena. As we will see, a promising approach is based on so-called phase-field methods, see Sec. *b* and inset *Phase-field models*.

a4) Experimental characterization and validation

The experimental reality of cavitation has often defied the predictive power of available models. For this reason, WP4 will support (with *validation* experiments) and guide (with *characterization* experiments) the other three theoretical/numerical units. In particular three main objectives are envisaged: **i) characterization of real nuclei and validation of nucleation models; ii) characterization of nuclei populations; iii) coalescence and collapse of bubbles**. In the following we briefly review the available techniques to achieve these objectives.

As already mentioned, nuclei are decisive in determining cavitation inception. For this reason, their shape has been characterized by Scanning Electron Microscopy (SEM) after filtration [34] and their observation in water has been pursued with a variety of methods [35]. On the one hand SEM allows for a precise geometric characterization of solid impurities once isolated from the liquid (this input will be used by WP1). On the other hand, **characterization of the nuclei populations within the working fluid is central for bridging the output of WP1 with WP2.** These latter experimental methods include a Venturi-based *cavitation susceptibility meter* [36], acoustic methods [37], phase-doppler techniques [38], light scattering and holography [39]. Nuclei populations may also be directly measured in the vicinity of the cavitating body [40] (e.g. a headform or a marine propeller).

The dynamics of bubble nucleation and growth from hydrophobic micropatterned crevices has been studied in [41] by imaging nucleation events induced therein by a pressure pulse. These experiments have been extended to nanopits fabricated with the aid of Focused Ion Beam (FIB) etching [42]. Targeted experiments similar to [41; 42] will be crucial in validating the heterogeneous nucleation models developed by WP1.

The recent development of high speed photography and microscopy allowed to capture the emission of water jets [30] and shock-waves [31] from a bubble collapsing near a solid wall. Similar techiques could be used to validate the results of WP3, in particular, bubble coalescence and collapse.

a5) Objectives & impact

The BIC project ambitious objective is to develop multiscale models and simulation techniques for cavitation, capable of predicting nucleation rates as well as bubble dynamics, deformation, and collapse in realistic flow conditions. From the picture provided in the previous paragraphs emerges that a thorough description of cavitation must embrace a multiplicity of scales and phenomena, to be addressed with an equally multifarious assortment of tools. The development and integration of such tools is the main objective of the BIC project. **The broad expertise in simulation techniques, ranging from advanced molecular dynamics to particle-laden turbulence, makes the PI especially suited for this task.** The reward for this ambitious objective would be the availability to the engineering community of predictive models for cavitation, ranging from nucleation to the stress induced on solid boundaries. In case of success, the BIC project would have a ground-breaking impact in the **design of turbomachinery, marine propellers, hydraulic structures** by supplying the models for realistically simulating cavitating flows across scales. In addition to these more traditional applications, another engineering field where accurate prediction of cavitation inception may have far-reaching consequences is the design of **Diesel injector nozzles** [43; 44].

An indirect, but not less important, impact of the BIC project will be on **ultrasound medicine**, that exploits acoustic cavitation for noninvasive therapies (e.g. High Intensity Focused Ultrasound -HIFU- therapy) and effective drug delivery [45-47]. As an example, HIFU therapy is emerging in the ablation of solid tumors [46], as the micro-bubble collapse induced in tissues by ultrasounds is capable of heating and destroying the tumorous cells *in-situ* without the need of surgery; accurate models for the nucleation process may suggest safer, more selective and efficient ways to induce and control cavitation in HIFU therapy. The extreme temperatures and pressures realized in collapsing bubbles, of the order of thousands of Kelvins and atmospheres [48], are also exploited in **sonochemistry** [49] (e.g. for ultrasound synthesis of nanomaterials [50; 51]) and in the realization of **chemical reactors based on hydrodynamic cavitation** [52; 53]. These promising new applications could greatly benefit from the tools developed along the BIC project. In particular, hydrodynamic cavitation reactors include all the scales considered in the project and their design would be more effective and economical if predictive models were available.

Furthermore each single work-package is expected to provide cutting-edge contributions to the specific area of concern, among others: **advanced models for nucleation mechanisms and rates, accurate description of the effects of turbulent transport on bubbles, bubble deformation and collapse via (compressible) phase-field models**, see Fig. 1.

Section b. Methodology

Project BIC is organized into four closely interacting work-packages (WPs) that will deal with different aspects and scales of cavitation:

1. WP1: Nucleation mechanisms and nucleation rate
2. WP2: Turbulent transport and bubble dynamics
3. WP3: Bubble deformation, topological changes, and collapse
4. WP4: Experimental characterization and validation

These WPs will work in parallel, but the work-load of each one will vary along the years, see Fig. 3. For instance, WP2 will be required to develop from the very beginning a coupled description of bubble-flow interactions, but, as nucleation models become available from WP1, the commitment of WP2 will increase. In general, as more tools become available from the theoretical/numerical WPs, the effort in integrating them into a comprehensive model will also increase. This is reflected in the progressive strategy used to allocate human resources, in particular PhD students, see Fig. 3 and Sec. *c*. The envisaged order of completion is WP1, WP2, and WP3 which allows for a better integration of the work-flow.

Work-package	Objective	M 1-6	M 7-12	M 13-18	M 19-24	M 25-30	M 31-36	M 37-42	M 43-48	M 49-54	M 55-60
WP1	Free energy simulations	RTD1 + PhD1 + [illegible]							RTD1		
	CRTI simulations	RTD1 + PhD1 + [illegible]							RTD1		
	TPT + TST						RTD1 + [illegible]				
WP2	DNS of turbulence	RTD2 + Senior1									
	One-way coupling	RTD2 + PhD2 + Senior1									
	Two-way coupling					PhD2 + Senior1				Senior1	
WP3	Phase-field simulations	Senior2									
	Compressible models					Senior2 + PhD3				Senior2 + PhD3	
	Collapse									Senior2 + PhD3	
	SEM on impurities										
	Nucleation on etched Si	RTD3									
	Nuclei in water										
	High speed photography										

Figure 3: Timing of the intermediate project objectives and distribution of human resources (Sec. c) for each project WP and specific objectives. Six months units are used, color code identifies the degree of commitment at a given time.

The interactions among the four WPs are schematized in Fig. 4 that shows intermediate objectives of each WP, supporting experiments by WP4, and milestones at the interface of WPs. In order to optimize communication between WPs and realize a truly interdisciplinary approach to cavitation, common milestones are envisaged. Milestones imply that different intermediate solutions will be screened by each WP (e.g. the numerical techniques used for nucleation, bubble transport, and bubble collapse) and validated experimentally by WP4. Milestones will be instrumental for defining the most appropriate solution both for describing the physics (does the model reproduce accurately enough the phenomenon?) and to interact with the next level of the phenomena (e.g. how can nucleation be incorporated into flow description?). This organization of the work-flow is crucial in order to achieve the most ambitious objective of the project, that is a coherent description of cavitation capable of bridging the different scales involved.

In the following we discuss in more detail the methods and work-plan envisaged for each work-package.

<u>*WP1: Nucleation mechanisms and nucleation rate*</u>

The problem of cavitation nuclei will be tackled with techniques unusual in engineering contexts, by exploiting the expertise acquired by our group in studying superhydrophobic surfaces [7, 8]. In particular, we propose to reconstruct the free energy profiles of the nucleation process of vapor cavities via **molecular dynamics free energy methods**, such as that devised in [54], that have already proved successful in describing the wetting/drying of surface crevices, see Fig. 5A and Ref. [7]. These simulations yield, for nanometer-sized particles and crevices having arbitrary geometry, information about the thermodynamic stability of the nucleus as a function of the liquid pressure and about the free energy barriers that need to be

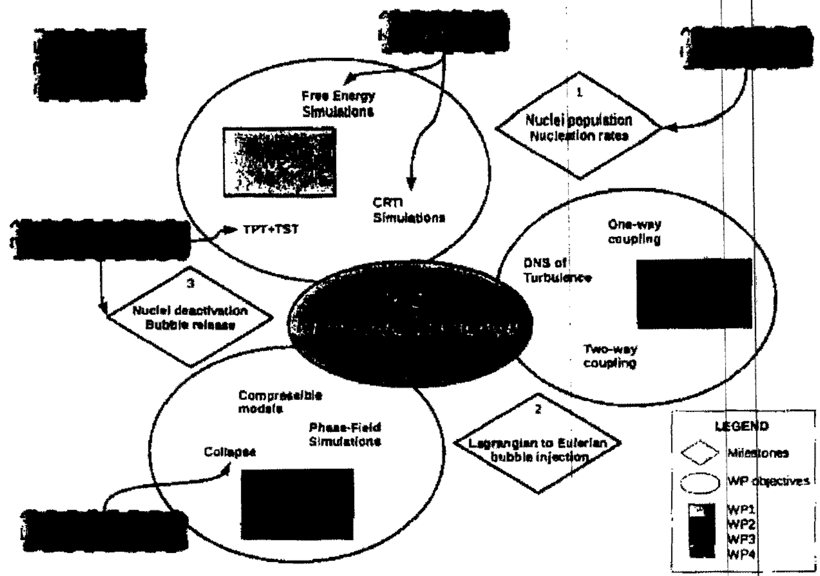


Figure 4: *Main objectives of BIC project organized by WPs. Milestones at the interface between WPs are meant to improve exchange of information between them and promote the main objective of the project* (in blue). In orange and dashed line, *the tasks of the experimental WP4.*

overcome i) for a nucleus to form and ii) for the nucleus to grow out of the crevice. Complementary to this atomistic approach is the Continuum Restrained Thermodynamic Integration (CRTI) proposed in [8] that allows to reconstruct free energy profiles also in a continuum framework. Practically CRTI extends the powerful atomistic description of nucleation to any particle or crevice in the nanometer to millimeter range, see Fig. 5B. An intermediate objective in the first phase of WP1 is the development of flexible and powerful algorithms that implement CRTI and the extension of this model to account for the effect of dissolved gas. After this objective will be achieved, realistic geometries of impurities typically present in engineering fluids could be simulated, based on the results of WP4, which will perform Scanning Electron Microscopy (SEM) analysis of solid impurities filtered from the liquid environment, see Fig. 4.

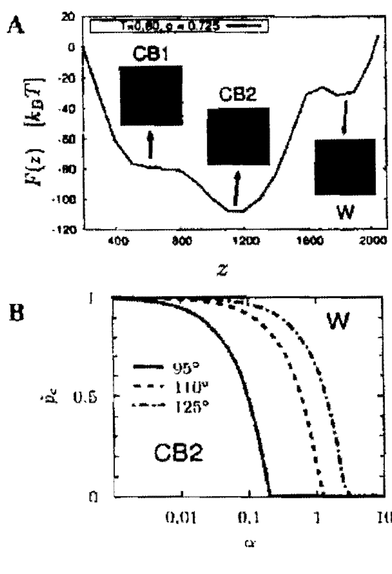


Figure 5: *A) Free energy profile as a function of the filling level of a single rectangular crevice z. In blue the liquid phase, in red the vapor phase of a simple fluid (Lennard-Jones). Local minima in the profile identify stable (absolute minimum) and metastable states (relative minima) in the wetting of a crevice. For the thermodynamic conditions represented, a nucleus with low curvature is the stable state (CB2), but other metastable states characterized by high curvature (CB2) and fully wet crevice (W) are also possible. The free energy barrier separating CB2 and W states is evident; such barriers confine the dynamics of the system within local minima, and only uncommonly high fluctuations may overcome them. For this reason nucleation on a rough surface is a* rare event *and its description requires advanced simulation techniques. The figure illustrates the restrained molecular dynamics simulations of* [7]. *B) Coexistence pressure (defined as the pressure where the probability of nucleation, i.e. of having a CB state, is ½) as a function of the crevice aspect ratio α (length over depth), for different contact angles (log-scale on abscissas). Data from the CRTI theory of* [8].

Robust thermodynamic models capable of describing i) nuclei stability and ii) free energy barriers as a function of the local pressure conditions will be the first step towards a rigorous theory of heterogeneous nucleation on rough surfaces (surface nuclei) and particles (free nuclei). Further improvement of the theory requires the knowledge of **the transition path and of the kinetics of the nucleation process.** In order to do this, we will employ the tools offered by transition path theory (TPT) [55] and transition state theory (TST) [56], which yield both the transition path and the nucleation rates. The models developed for nucleation will be validated on simple crevice geometries (e.g. cylindrical ones) against *ad-hoc* experiments on micro-patterned surfaces carried out by WP4, similar to those in [42]. In this phase, interaction with the phase-field description of WP3, assisted by the targeted experiments of WP4, will provide insights in the bubble release process and the nuclei deactivation mechanism proposed in [42], see Milestone 3 in Fig. 4.

The outlined approaches will allow a rigorous description of the nucleation process on known surface asperities and indeed may represent a significant advancement for the field of nucleation. However in practical situations a plethora of nuclei having different geometries and surface characteristics are present. Therefore, in order to interact with the subsequent step of the multiscale description, models for the nuclei population are needed, see Milestone 1 in Fig. 4. These models will be developed interacting with the experimental unit WP4 that is in charge of characterizing the nuclei populations in different liquids.

WP2: Turbulent transport and bubble dynamics

WP2 is in charge of developing fast and accurate algorithms for the transport of cavitation nuclei and of the bubbles in the stage when they are too small to be resolved on the grid of the Navier-Stokes solver. In these conditions, nuclei (both those freely advected by the fluid and those existing on the rough surface of the immersed body) and bubbles are considered as point particles endowed with different dynamical features (internal degrees of freedom). The concept is a combined Eulerian-Lagrangian approach (for fluid and particles, respectively) to track the generalized particles in a fully resolved turbulent flow in the spirit of Direct Numerical Simulation (DNS). The nuclei will be equipped with an activation rate model according to the heterogeneous nucleation theory developed in WP1, see Fig. 4. The sub-Kolmogorov bubbles will be endowed with a geometrical descriptor (the bubble radius in the simplest case, but a variety of simple shape parameters related to the bubble deformation will also be considered) and will evolve according to a generalized Rayleigh-Plesset dynamics (see inset *The Rayleigh-Plesset Equation)*. During the first stage of the project, while waiting for the results of WP1, the focus will be held on bubble description.

The truly innovative advancement expected from WP2 is the effective coupling of cavitation nuclei and bubbles with the turbulent flow. On the one hand, nuclei and bubbles will perceive the local instantaneous pressure history along their own turbulent Lagrangian trajectories. In such conditions the local pressure will drive the evolution of the particle internal degrees of freedom (e.g. the bubble radius or the nucleation rate on free nuclei) while convected by the turbulent flow (*one-way coupling*). On the other hand, bubbles will modify their micro-environment through momentum, heat, and mass exchange with the fluid and affect the flow via collective effects (*two-way coupling*). **The most innovative outcome of WP2 is indeed developing accurate and fast algorithms, able to track millions of particles in the particularly severe conditions of**

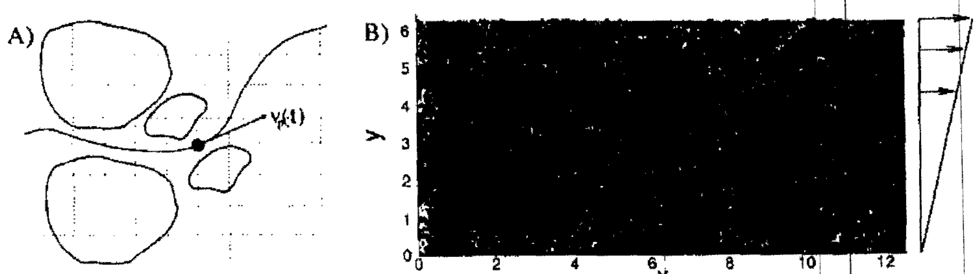


Figure 6: *A) Sketch of the two-way coupling algorithm. The red lines show the vorticity injected on the grid during the time step on few nodes around the particle influenced. The vorticity already present on the Eulerian grid is evolved by the Navier-Stokes solver* (green lines). *At each time step new vorticity is injected on the grid, to be successively taken care by the N-S solver. B) Instantaneous particle configurations (black dots) superimposed to the isolines* (colors) *of the newly injected vorticity. The simulation is a fully turbulent 3D, particle-laden homogenous shear flow* (from [57]).

two-way coupling. The concept exploits the small Reynolds number of the local relative fluid-particle velocity. In these conditions diffusive processes dominate over convection, allowing to approximate convection as a second order effect. Restricting, for the sake of definiteness, the attention to momentum coupling, the particle reacts on the fluid with the opposite force the fluid is exerting on the particle (essentially the Stokes drag, see the inset *The Maxey-Riley equation).* With respect to the standard approach followed for two-way coupling simulations that employ the steady state Green's function for diffusion [58], the ground-breaking increase of computational efficiency is expected to come from describing diffusion (of momentum, in this specific example) in an intrinsically time-dependent framework, using the so-called free-space Green's function of the unsteady diffusion operator. Given the narrowly peaked shape of the unsteady Green's function at small time delays (a Gaussian with variance proportional to the time step), the time stepping procedure couples the particles with the discrete Eulerian field only though a few grid nodes around the particle, see Fig. 6A. This opens the way to a new class of algorithms for the diffusion-dominated coupling of particle ensembles with Eulerian fields. Their complexity scales *linearly* with the number of transported particles, making them potentially able to simulate turbulent flows with millions of transported bubbles, see Fig. 6B.

In a fundamental study such as that proposed in BIC project, use of DNS is strategic in order to reconstruct the correct physical mechanism of bubble-flow interactions. The DNS simulation of practical engineering flows, however, is beyond current computational capabilities. In a late phase of the BIC project, WP2 resources will be devoted implement the obtained results into Large Eddy Simulation (LES) sub-grid models, so as to supply practical computational tools to the engineering community.

WP3: Bubble deformation, topological changes, and collapse

Once a bubble has grown to a size comparable with the Kolmogorov scale, it can be resolved on the Eulerian grid. The subsequent phase of extreme bubble deformation, merging and collapse in presence of shock waves emission, solid boundaries, and real turbulence is out of the reach of any presently available simulation technique. **To bridge this gap towards the actual multiscale description of turbulent cavitation a radically innovative approach based on the so-called diffuse interface (or phase-field) methods** [59] (see also inset *Phase-field methods*) is here envisaged. As explained in further detail in the inset, this approach has the potential to track the evolution of the bubbles in the turbulent field, allowing for extreme deformations of the bubble shape, for topological rearrangements, such as merging of two or more bubbles, and for flow-induced bubble break-up. In a nutshell, the basic concept is replacing the sharp interface between a bubble and surrounding liquid with a diffuse interface across which the fluid properties change smoothly from the values pertaining to the liquid outside the bubble to those pertaining to the gaseous state inside the bubble [60]. A preliminary example of its potential is provided in Fig. 7, showing the evolution of an enclosure of a fluid immiscible with the background liquid, like an oil drop in water. Both flows inside and outside the bubble are resolved, allowing the implicit correct tracking of the enclosure. We recently succeeded in theoretically showing, and numerically confirming, the convergence of the diffuse interface description to the correct sharp interface limit where the smooth interfacial layer approaches the appropriate jump conditions at the surface enclosure [61].

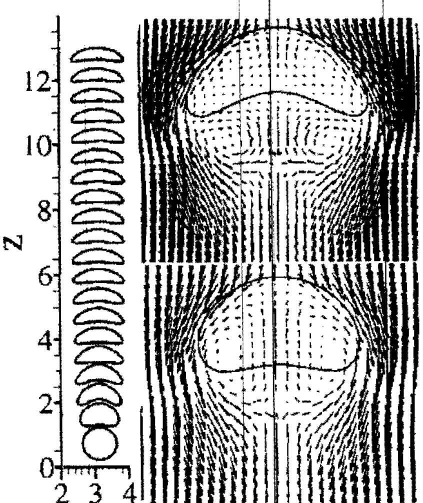


Figure 7: A) Rising bubble in a liquid under buoyancy forces. B) Instantaneous configurations of bubble interface (solid line) and fluid velocity (arrows). Three-dimensional simulation with phase-field model [62].

The approach can be endowed with rigorous thermodynamics to describe the liquid-vapor phase transition. The isothermal assumption, see the inset, can be relieved by introducing the energy equation, e.g. in terms of the temperature field. The approach features a state equation for the bulk phases encompassing both vapor and liquid states. The liquid compressibility is kept in the liquid equation of state so as to support acoustic and shock wave propagation, in view

Phase-field methods

Starting from the pioneering work of van der Waals [60], two phase fluids (vapor bubbles immersed in the liquid, in our case) have been described by a *free-energy functional*

$$F[\rho,T]=\int_D f(\rho,\nabla\rho,T)dV\approx\int_D[f_b(\rho,T)+1/2\lambda(T)\nabla\rho\cdot\nabla\rho]dV \ ,$$

where $\rho(x,t)$ is the continuously varying density field, T the temperature, here assumed constant for simplicity, and D the flow domain. The free-energy density f is the sum of the *bulk* free-energy of the pure fluid f_b –typically the free-energy of a van der Waals fluid– and an *interfacial* term proportional to the squared density gradient. Equilibrium conditions are solutions of the Euler-Lagrange equations which determine the minima of the (locally) convex functional constrained to a given mass of the system, $\delta F/\delta\rho=\partial f_b/\partial\rho-\lambda\nabla^2\rho=\mu_0$, where μ_0 is the Lagrange multiplier used to enforce the mass constraint. The functional derivative $\mu=\delta F/\delta\rho$ is the chemical potential that is constant at equilibrium. The solution of the resulting non-linear elliptic equation determines the equilibrium density field $\rho_{eq}(x)$. Below the critical temperature the bulk free-energy density ceases to be a globally convex function of the density, and the equilibrium density field features two bulk states $\rho_l>\rho_v$, corresponding to liquid and vapor, respectively. The two phases are separated by a thin transition region, the so-called *diffuse interface*. Equilibrium is the results of two competing effects, namely segregation in two distinct phases, towards by the two identical minima in the bulk grand-potential $\omega_b=f_b-\mu_0\rho$, and reduction of the interface, penalized by the interfacial energy.

Under non-equilibrium conditions the field is assumed to relax towards equilibrium along the steepest descent trajectory. Beside the mass conservation equation,

$$\frac{\partial\rho}{\partial t}=-\nabla\cdot(\rho\boldsymbol{u}) \ ,$$

tthe momentum conservation

$$\frac{\partial\rho\boldsymbol{u}}{\partial t}+\nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u})=\nabla\cdot\boldsymbol{T}_\pi+\nabla\cdot\boldsymbol{T}_\mu$$

includes, in addition to the standard viscous term $\boldsymbol{T}_\mu$, the extra-stress $\boldsymbol{T}_\pi=\boldsymbol{T}_\pi[\rho]$ corresponding to a distributed capillary stress across the interface [59]. Its form is too cumbersome to be explicitly reported here. It could however suffice to say that it is a functional of the density that basically contains square terms in the density gradient and the bulk chemical potential, $\mu_b=\partial f_b/\partial\rho$, related to the thermodynamic pressure. Once integrated across the interface, the capillary stress provides the surface tension and the stress difference between the two bulk phases. For isothermal flows the above two equations completely determine the dynamics, including the liquid/vapor phase transition that may occur in response to changes in the bubble environment. Clearly, when the Reynolds number is large enough, the flow becomes turbulent, inheriting all the rich thermodynamics of the liquid/bubble interactions. The field naturally accommodates for topological rearrangements of the bubbles, i.e. flow-induced bubble merging and fragmentation. Interestingly, the bulk equation of state for pressure derived from the bulk free-energy density keeps compressibility effects, both in the vapor and in the liquid phase. As a last note, the formulation can be extended to non-isothermal conditions with a suitable form of energy equation dependent on the temperature field $T=T(x,t)$.

of the correct evaluation of the stress induced on a solid wall by the collapse of cavitation bubbles.

It is finally worth stressing that WP2 and WP3 will operate on the same common Navier-Stokes platform and that a procedure to smoothly shift on-the-fly from a particle based to a phase-field description is envisaged, see Milestone 2 in Fig. 4. A new algorithm will be devised to guarantee seamless injection of Lagrangian bubbles into the phase-field description on the Eulerian grid. **In this sense the BIC project will possibly achieve its most high-risk but at the same time most rewarding objective of providing integrated simulative tools to rigorously bridge the range of scales from nucleation to bubble transport (WP1→WP2) to topology change and eventual collapse (WP2→WP3).**

WP4: Experimental characterization and validation

Experimental methods will serve both as a support for validating the models developed by the other WPs and for characterizing realistic nucleation scenarios, see Fig. 4. In order to perform these tasks, **we plan to use flexible and versatile techniques, capable to adapt to the project evolution and adjustments**. For micro- and nanocharacterization and fabrication BIC project will greatly benefit from the facilities available at the Sapienza *Research Center for Nanotechnologies Applied to Engineering* (CNIS). The proponent is member of the steering committee of CNIS and his research group has access to the resources therein. The facilities at CNIS include a high resolution field emission SEM, equipped with Electron-Beam Lithografy (EBL), Energy Dispersive X-ray Spectroscopy (EDS), and Focused Ion Beam (FIB), two Atomic Force Microscopy (AFM) platforms, a confocal fluorescence microscope, chemical vapor deposition (CVD) system, and chemical lab. A class 1000 clean room is available at the Department of Information, Electronic and Telecommunication Engineering (DIET) of Sapienza. Other equipment will be acquired in the course of the project, to allow optical and acoustical characterization of nuclei and bubbles. A possible experimental setup will include a light source (e.g. laser or strobo), lenses and optics (microscope etc.), high-speed camera, hydrophone, and pressure control. The specifications of these additional instruments will become clear in a later phase of the project, when the final design of the experiments will be possible based on the intermediate results of the other WPs. Further details on the available and planned experimental resources are described in Sec. *c*.

With the just described equipment, the methodologies that can be envisaged in this phase are (see Fig. 4):

1. SEM characterization of typical solid impurities isolated from water, including geometry and chemistry (via EDS). This will yield realistic models for solid cavitation nuclei as inputs for WP1.
2. Realization of micro and nanopatterned surfaces of controlled size and geometry via FIB and EBL techniques. Deposition of hydrophobic layers via Chemical Vapor Deposition (CVD), as already done, e.g., in [64]. Determination of the cavitation pressure on the realized crevices with the methods of [41; 42], which are essentially based on imaging the nucleation event triggered by a pressure pulse. These methods will be helpful in validating the nucleation models of WP1.
3. Characterization of nuclei populations in water via light scattering or holographic techniques [35]. The final method will be selected depending on the project needs and the versatility of the equipment. These experiments will be useful to supply nuclei population models as inputs for WP2.
4. Characterization of bubble coalescence and collapse at solid walls. The second task may require high-speed photography [30; 31] and will be considered in the final phase of the BIC project, as a validation of WP3 high-risk task of simulating via phase-field compressible models bubble collapse, see Fig. 1.

Section c. Resources

c1) Personnel

The BIC project is a chiefly theoretical and numerical project, that involves the development of new numerical approaches in many diverse areas. For this reason most of the project resources will be devoted to hiring experienced researchers, capable of proposing cutting-edge solutions in each area of the research (embodied by the WPs).

The PI commitment to BIC project will be the 50% of his working time, as a close supervision of the four WPs (that work mostly in parallel, see Figs. 3 and 4) is intended to promote a unified vision to the project. The cost of the PI is 100 000 €/year.

In addition to the PI, Dr. P. Gualtieri, assistant professor at the Department of Mechanical and Aerospace Engineering Department of Sapienza, will actively help coordinating the numerical effort of the project. His expertise in DNS of particle-laden flows, in one-way [18] and two-way coupling [57] regimes makes him especially suited for leading WP2. He is expected to devote 60% of his working time to the BIC project. The cost of an assistant professor is around 50 000€/year. Prof. Luca Marino, associate professor at the Mechanical and Aerospace Engineering of Sapienza, will contribute to the development of phase field models. His expertise in the field of compressible flows and phase field models will help with WP3. The cost of an associate professor is around 70 000€/year. He will be involved for 50% of his working time.

The other WPs will also be led by experienced researchers, more specifically associated professors and post-docs (in the Italian regime Ricercatori a tempo determinato di tipo A, RTD-A) already acquainted with the methods envisaged for their WP: rare events methods for WP1, Direct Numerical Simulation for WP2, and experimental methods for WP4. **A total of three RTD-A will be hired in the first months of BIC project for the whole duration of it, and they are expected to work full-time for the project.** This strategy will allow the WPs to be fully operative in the first year of the project. The current cost of a RTD-A is around 50 000 €/year in Italy.

At least four PhD students will be formed and work on the BIC project. In addition to state-funded PhD scholarships, dedicated ones may be awarded. In the first year, WP1 is required to provide rapidly basic nucleation models to WP2; in order to do this a PhD student will work on WP1. From the beginning, another PhD will be employed in WP4, in particular, to design and build the experimental setup not already at CNIS center. At least two PhD students will join the BIC project in successive years, to support the effort of integrating WPs work. One is expected to help WP2 from the second year of the project. The other will help WP3 starting in the third year. The cost of a **three year PhD scholarship** is around 48 000€ in Italy; PhD positions are announced once a year in September.

In order to deal with the experimental part of WP4 experienced technicians are needed. Technical personnel is also required to manage the computer resources. The related expenses are reported as Other Personnel Costs in the table attached below.

Appropriate resources will be devoted to promote research travels for each category of the research staff, including participation to international conferences. In particular, each PhD student will be encouraged to spend in a European university an average of six months, to perfect specialized aspects of her/his research. Hosting of visiting researchers and PhD students will also be promoted, as a means to enrich the expertise available to the BIC project and to disseminate its results.

c2) Existing resources

The facilities available at CNIS center of Sapienza will be exploited along the five years for micro- and nanofabrication and characterization. An annual membership fee of 4000€ allows members of the research group to use the available equipment for around 1000 hours and obtain technical support. In particular, we are interested in the Auriga Zeiss High Resolution FESEM platform that has also modules for spectrography (EDS *Bruker*) and nanofabrication (EBL *Reith* and FIB). This platform will allow to characterize the solid particles typically present in water residue, to etch silicon and other materials, and to characterize the etched micro- and nanoholes. A complementary technology for nanocharacterization also present at CNIS is Atomic Force Microscopy (AFM *Veeco Multimode* and *Veeco Icon*). Chemical vapor deposition system (e.g. for depositing hydrophobic layers) and a chemical lab are also present at CNIS center. A class 1000 clean room is available at the Department of Information, Electronic and Telecommunication Engineering (DIET) of Sapienza with which the PI has an ongoing collaboration [64].

c3) Equipment

New experimental setups will be acquired in order to characterize i) nucleation on micro- and nanopatterned surfaces, ii) nuclei in water, and iii) bubble collapse. In order to effectively support the work of the other WPs, flexible instrumentation will be preferred. Possible solutions for the fluidic setups are listed in the following.

An optical table, microscope, light source (strobo or LASER), and pressure control (e.g. a piezoelectric source as in [41]) will allow to realize i). Subsequently few additional equipment is needed for ii), e.g. a different light source [35]. In the last two years, in addition to the accumulated equipment, a high-speed camera and possibly hydrophones will be needed to perform iii).

Generous computational resources will also be needed. These resources will be made available through high-performance computing centers. Typical cost for 100 000 computational hours (either on HPC or GPU clusters) and 1 terabyte of storage is around 10 000€ (as estimated from the group's contracts with CASPUR/CINECA). An average consumption of 200 000 hours/year is expected on traditional clusters and 100 000 hours/year on GPUs. A portion of these resources may be provided through the acquisition of computational/GPU clusters. The costs concerning the computational resources are budgeted in the table attached below under the entry *Equipment*, as concerning the acquisition of local clusters. The part concerning the computational hours to be used on CINECA supercomputers is budgeted instead under the entry *Consumables*.It may be worth specifying that in both cases the PI and the personnel involved in the project will work in the premises of the host institution, using in case online connections to the supercomputer centre. Of the required 300 000 computational hours/per year, the share is order 57% spent on the local clusters and 43% on the CINECA machines. It can be anticipated that along the project it could be necessary to partially adjust such percentages and the corresponding allocated budget.

c4) Travel expenses for external experts and dedicated workshops

Short visiting periods are envisaged for external experts to be selected according to the specific needs of the project. Two workshops are foreseen, one during the first accounting period and one during the third one, with the purpose of gathering together worldwide experts in the different fields of cavitation in order to focus project towards the issues suggested as crucial by the scientific community.

c5) Consumables, Publications and Subcontracting

Consumables. The BIC projects will mainly use two different kinds of consumables. On the one end the experimental work-package WP4 will employ consumables of different nature to accomplish the SEM characterization of impurities (item 1 of WP4), the realization of micro/nano patterned surfaces (item 2 of WP4), the characterization of nuclei population in water (item 3 of WP4), the characterization of bubble coalescence and collapse at solid walls (item 4 of WP4). On the other hand, the extensive computational activity of the project will use typical consumables associated with the use of PC-clusters, hard-disk storage systems and similar items. Consumables include also the annual membership fee for accessing the CNIS facilities and, as anticipated before, the cost of computer hours to be used on CINECA supercomputers.

Publications. The scientific results achieved during the different phases of the BIC project will we made publicly available through publication in open access journals. In several cases costs are attached to this kind of publications that will be financed through the BIC grant.

Subcontracting. Some funding will be needed for subcontracting. Among these are worth mentioning here the costs of external audits to keep the financial part of the project under strict control and the realization of micro-nano patterned surfaces for the experimental study of nucleation.

ERC C.1 INTERNAL USE

ERC Advanced Grants **339446 BIC**

Budget tables to be inserted in section c) "Resource", heading III. "Budget"

III. Budget - Table 1 [redacted] **60**

	Cost Category	month 1 to 18	month 19 to 36	month 37 to 54	month 55 to 60	Total
Direct Costs:	**Personnel:**					
	PI [2]	75.000,00	75.000,00	75.000,00	25.000,00	250.000,00
	Senior Staff	80.000,00	80.000,00	80.000,00	26.000,00	266.000,00
	Post docs	225.000,00	225.000,00	225.000,00	75.000,00	750.000,00
	Students	48.000,00	72.000,00	48.000,00	8.000,00	176.000,00
	Other	10.000,00	10.000,00	10.000,00	3.000,00	33.000,00
	Total Personnel:	**438.000,00**	**462.000,00**	**438.000,00**	**137.000,00**	**1.475.000,00**
	Other Direct Costs:					
	Equipment	57.000,00	57.000,00	57.000,00	19.000,00	190.000,00
	Consumables	35.000,00	35.000,00	35.000,00	5.000,00	110.000,00
	Travel	50.000,00	55.000,00	55.000,00	10.000,00	170.000,00
	Travel costs for international experts	15.000,00	7.000,00	15.000,00	5.000,00	42.000,00
	Publications	10.000,00	10.000,[illegible]	10.000,00	2.850,00	32.850,00
	Workshop	[illegible]	[illegible]	15.000,00		30.000,00
	Total Other Direct Costs:	**182.[illegible]**	**164.000,[illegible]**	**187.000,00**	**41.850,00**	**574.850,00**
	Total Direct Costs:	**[illegible].000,00**	**626.000,00**	**625.000,00**	**178.850,00**	**2.049.850,00**
Indirect Costs (overheads):	20% of Direct Costs	124.000,00	125.200,00	125.000,00	35.770,00	409.970,00
	20 % cs	*124.000,00*	*125.200,00*	*125.000,00*	*35.770,00*	*409.970,00*
Subcontracting Costs:	(No overheads)	15.000,00	11.500,00	4.000,00	880,00	31.380,00
Total Requested Grant:	(by reporting period and total)	**759.000,00**	**762.700,00**	**754.000,00**	**215.500,00**	**2.481.200,00**

Page 1

[1] Adapt to actual project duration.
[2] Please take into account the percentage of your dedicated working time (minimum 30%) to run the ERC funded activity when calculating the salary

For the above cost table, please indicate the % of working time the PI dedicates to the project over the period of the Grant :	50,00%

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Section d. Ethical and security-sensitive issues

ETHICS ISSUES TABLE

Areas Excluded From Funding Under FP7 ***(Art. 6)***

(i) Research activity aiming at human cloning for reproductive purposes;

(ii) Research activity intended to modify the genetic heritage of human beings which could make such changes heritable (Research relating to cancer treatment of the gonads can be financed);

(iii) Research activities intended to create human embryos solely for the purpose of research or for the purpose of stem cell procurement, including by means of somatic cell nuclear transfer;

All FP7 funded research shall comply with the relevant national, EU and international ethics-related rules and professional codes of conduct. Where necessary, the beneficiary(ies) shall provide the responsible Commission services with a written confirmation that it has received (a) favourable opinion(s) of the relevant ethics committee(s) and, if applicable, the regulatory approval(s) of the competent national or local authority(ies) in the country in which the research is to be carried out, before beginning any Commission approved research requiring such opinions or approvals. The copy of the official approval from the relevant national or local ethics committees must also be provided to the responsible Commission services.

Guidance notes on informed consent, dual use, animal welfare, data protection and cooperation with non-EU countries are available at :
http://cordis.europa.eu/fp7/ethics_en.html#ethics_sd

For real time updated information on Animal welfare also see:
http://ec.europa.eu/environment/chemicals/lab_animals/home_en.htm
For real time updated information on Data Protection also see: http://ec.europa.eu/justice/data-protection/index_en.htm

Research on Human Embryo/ Foetus	YES	Page[1]
Does the proposed research involve human Embryos?		
Does the proposed research involve human Foetal Tissues/ Cells?		
Does the proposed research involve human Embryonic Stem Cells (hESCs)?		

1 Please indicate here the page number of Part B2 of your proposal on which the ethical issue in question arises.

Does the proposed research on human Embryonic Stem Cells involve cells in culture?		
Does the proposed research on Human Embryonic Stem Cells involve the derivation of cells from Embryos?		
I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

Research on Humans	YES	Page
Does the proposed research involve children?		
Does the proposed research involve patients?		
Does the proposed research involve persons not able to give consent?		
Does the proposed research involve adult healthy volunteers?		
Does the proposed research involve Human genetic material?		
Does the proposed research involve Human biological samples?		
Does the proposed research involve Human data collection?		
I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

Privacy	YES	Page
Does the proposed research involve processing of genetic information or personal data (e.g. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)?		
Does the proposed research involve tracking the location or observation of people?		
I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

Research on Animals	YES	Page
Does the proposed research involve research on animals?		
Are those animals transgenic small laboratory animals?		
Are those animals transgenic farm animals?		
Are those animals non-human primates?		
Are those animals cloned farm animals?		
I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

Research Involving non-EU Countries (ICPC Countries[2])	YES	Page
Is the proposed research (or parts of it) going to take place in one or more of the ICPC Countries?		

2 In accordance with Article 12(1) of the Rules for Participation in FP7, 'International Cooperation Partner Country (ICPC) means a third country which the Commission classifies as a low-income (L), lower-middle-income (LM) or upper-middle-income (UM) country. Countries associated to the Seventh EC Framework Programme do not qualify as ICP Countries and therefore do not appear in this list.

	Is any material used in the research (e.g. personal data, animal and/or human tissue samples, genetic material, live animals, etc) : a) Collected and processed in any of the ICPC countries?		
	b) Exported to any other country (including ICPC and EU Member States)?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

	Dual Use	YES	Page
	Research having direct military use		
	Research having the potential for terrorist abuse		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

If any of the above issues apply to your proposal, you are required to complete and upload the 'B2_Ethical Issues Annex' (template provided).

Without this Annex, your application cannot be properly evaluated and even if successful the granting process will not proceed.
Please see the Guide for Applicants for the Advanced Grant 2013 Call for further details and CORDIS http://cordis.europa.eu/fp7/ethics_en.html for further information on how to deal with Ethical Issues in your proposal.

DIPARTIMENTO DI INGEGNERIA
MECCANICA E AEROSPAZIALE
IL DIRETTORE
(Prof. Giorgio Graziani)

SUPPLEMENTARY AGREEMENT
(Support for frontier research)

Università degli Studi di Roma La Sapienza, (hereinafter referred to as "*beneficiary*"),

of the one part,

Carlo Massimo Casciola, Italian, passport No. F 500501, (hereinafter referred to as *"principal investigator")*,

of the other part,

Have agreed to the following terms and conditions and fully accept the terms defined in the *grant agreement* (ERC *grant agreement* No. 339446), which have the same meaning in this *supplementary agreement*[1].

1. Scope of the *supplementary agreement*

The present *supplementary agreement* shall determine the conditions for implementing the project "Cavitation across scales: following Bubbles from Inception to Collapse" (hereinafter referred to as "*project*") and the respective rights and obligations of the *principal investigator* and the *beneficiary*. Provisions of this *supplementary agreement,* which are not in accordance with the *grant agreement*, shall be deemed to be void.

2. Rights and obligations of the beneficiary

The *beneficiary* shall:

1. support the *principal investigator* in the management of the *team* and provide reasonable administrative assistance to the *principal investigator*, in particular as regards:

    a. the timeliness and clarity of financial information,

    b. the general management and reporting of finances,

    c. the advice on internal *beneficiary* strategies and *ERC or Commission* policies,

    d. the organisation of *project* meetings as well as the general logistics of the *project.*[1]

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[1] *Grant agreement* means the ERC grant agreement including its annexes between the *beneficiary* and the *European Research Council Executive Agency (hereinafter referred to as the "Agency")* under the Seventh Framework Programme (FP7).

3. Rights and obligations of the principal investigator

The *principal investigator* shall:

1.

a) take all appropriate steps towards the effective supervision of the scientific and technological execution of the *project*;

b) be in charge of the scientific reporting and contribute effectively to the financial management reporting on the *project*;

c) inform the *beneficiary* in due time of any event or change in circumstances which are likely to have an effect on the performance of the *grant agreement*, inter alia:

- a planned transfer of the *project* to a new *beneficiary*;
- any modification relating to the information having served as a basis to the signature of the supplementary agreement referred to in Article 2 of the *grant agreement*;
- any modification relating to the information having served as a basis for the award of the ERC grant;
- any personal grounds affecting the implementation of the *project*.

d) respect the confidentiality rules in accordance with Article II.9 of the *grant agreement*.

e) acknowledge the support of the European Union for an ERC grant in any dissemination activities, such as in related publications or other media in accordance with Article II.12 of the *grant agreement*.

2. the *principal investigator* shall respect the intellectual property rights of the *beneficiary* during and after the *project*;

3. the *principal investigator* shall propose in writing to the *beneficiary* in the case he/she decides to transfer the *project* to a new beneficiary to which extent the *project* shall be transferred. He/she shall also make in writing a proposal to the *beneficiary* on the modalities of the transfer arrangement with the new *beneficiary*.

4. the *principal investigator* shall provide to the *beneficiary* in the case of transfer to the new *beneficiary* a statement describing in detail the results of the conducted research up to the time of transfer of the *project* and he/she shall transmit a copy of this statement to the *Agency*.

Grant Agreement Preparation Forms

Project number
339446

Project title
BIC— Cavitation across scales: following Bubbles from Inception to Collapse

Call (part) identifier
ERC-2013-ADG

Funding scheme
Support for frontier research (ERC)

A1:
Our project

Project Number [1]	339446	Project Acronym [2]	BIC

General information		
Project title [3]	Cavitation across scales: following Bubbles from Inception to Collapse	
Starting date [4]	01/02/2014	
Duration in months [5]	60	
Call (part) identifier [6]	ERC-2013-ADG	
Activity code [7]	ERC-AG-PE8 : ERC Advanced Grant - Products and process engineering	
ERC review panel(s) [53]	PE8	
Free keywords [8]		- Cavitation - Heterogenous nucleation - Rare events techniques - Molecular dynamics - Phase field methods - Bubble dynamics - Bubble collapse - Lagrangian tracking - Multiphase flows - Flow solver

Abstract [9] (max. 3000 char.)

Cavitation is the formation of vapor cavities inside a liquid due to low pressure. Cavitation is an ubiquitous and destructive phenomenon common to most engineering applications that deal with flowing water. At the same time, the extreme conditions realized in cavitation are increasingly exploited in medicine, chemistry, and biology. What makes cavitation unpredictable is its multiscale nature: nucleation of vapor bubbles heavily depends on micro- and nanoscale details; mesoscale phenomena, as bubble collapse, determine relevant macroscopic effects, e.g., cavitation damage. In addition, macroscopic flow conditions, such as turbulence, have a major impact on it.

The objective of the BIC project is to develop the lacking multiscale description of cavitation, by proposing new integrated numerical methods capable to perform quantitative predictions. The detailed and physically sound understanding of the multifaceted phenomena involved in cavitation (nucleation, bubble growth, transport, and collapse in turbulent flows) fostered by BIC project will result in new methods for designing fluid machinery, but also therapies in ultrasound medicine and chemical reactors. The BIC project builds upon the exceptionally broad experience of the PI and of his research group in numerical simulations of flows at different scales that include advanced atomistic simulations of nanoscale wetting phenomena, mesoscale models for multiphase flows, and particle-laden turbulent flows. The envisaged numerical methodologies (free-energy atomistic simulations, phase-field models, and Direct Numerical Simulation of bubble-laden flows) will be supported by targeted experimental activities, designed to validate models and characterize realistic conditions.

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A2.1:
Who we are

Project number[1]	339446	Project acronym[2]	BIC	Host Institution number in this project[10]	1	Host Institution short name[11]	Uniroma1

One form per participant

Legal data

If your organisation has already registered for FP7, enter your Participant Identity Code[12]	999987745
Participant legal name[13]	UNIVERSITA DEGLI STUDI DI ROMA LA SAPIENZA
Participant short name[11]	Uniroma1
Status of validation[14]	VALID

Legal address of the participant			
Street name[15]	Piazzale Aldo Moro 5	Number[15]	
Town[15]	ROMA		
Postal code / Cedex[15]	00185		
Country[16]	Italy		
Internet homepage (optional)	www.uniroma1.it		

Registration data of the participant	
Legal registration number[17]	80209930587
Place of registration[17]	N/A
Date of registration[17]	29/07/1982
VAT number[18]	IT02133771002
Legal form[19]	UNK

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A2.3: Authorised Representatives

Project number [1]	339446	Project acronym [2]	BIC	Host Institution number in this project [10]	1	Host Institution short name [11]	Uniroma1

One form per participant

Authorised representative to sign the grant agreement or to commit the organisation for this project			
Family name	Graziani	First name(s)	Giorgio
Title [34]	Prof.	Gender [35] (Female – F / Male – M)	M
Position in the organisation [36]		Director of Mechanical and Aerospace Engineering Department	
Department/Faculty/Institute/Laboratory name/... [37]		Mechanical and Aerospace Engineering Department	
Address (if different from the legal address) [12]			
Street name [15]	via Eudossiana	Number [15]	18
Town [15]	Roma		
Postal code / Cedex [15]	00184		
Country [16]	Italy		
Phone 1 [21]	+390644585266	Phone 2 [21]	+393201891341
E-mail	g.graziani@uniroma1.it	Fax [21]	+390644585250

Alternative authorised representative to sign the grant agreement or to commit the organisation for this project			
Family name		First name(s)	
Title [34]		Gender [35] (Female – F / Male – M)	
Position in the organisation [36]			
Department/Faculty/Institute/Laboratory name/... [37]			
Address (if different from the legal address) [12]			
Street name [15]		Number [15]	
Town [15]			
Postal code / Cedex [15]			
Country [16]			
Phone 1 [21]		Phone 2 [21]	
E-mail		Fax [21]	

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A2.5: Our commitment

Project number[1]	339446	Project acronym [2]	BIC	Host Institution number in this project [10]	1	Host Institution short name [11]	Uniroma1

One form per participant

Certified declaration

1- As an authorised representative to sign the grant agreement or to commit the abovementioned organisation, I am fully aware that a grant agreement may not be awarded to an applicant who is, at the time of a grant award procedure, in one of the situations referred to in Articles referred to in Articles 106(1), 107 and 109(2)(a) of the Regulation (EU, Euratom) No 966/2012 of the European Parliament and of the Council of 25 October 2012 on the financial rules applicable to the general budget of the Union and repealing Council Regulation (EC, Euratom) No 1605/2002 [OJ L298, 26.10.2012, p.1].

As a consequence, I certify that:

- In compliance with article 106(1) of the abovementioned Regulation, none of the following cases apply to our organisation:
  a) it is bankrupt or being wound up, is having its affairs administered by the courts, has entered into an arrangement with creditors, has suspended business activities, is the subject of proceedings concerning those matters, or is in any analogous situation arising from a similar procedure provided for in national legislation or regulations;
  b) it or persons having powers of representation, decision making or control over it have been convicted of an offence concerning their professional conduct by a judgment which has the force of res judicata;
  c) it has been guilty of grave professional misconduct proven by any means which the contracting authority can justify including by decisions of the EIB and international organisations ;
  d) it is not in compliance with its obligations relating to the payment of social security contributions or the payment of taxes in accordance with the legal provisions of the country in which it is established or with those of the country of the contracting authority or those of the country where the contract is to be performed;
  e) it or persons having powers of representation, decision making or control over it have been the subject of a judgment which has the force of res judicata for fraud, corruption, involvement in a criminal organisation or any other illegal activity, where such illegal activity is detrimental to the Union's financial interests;
  f) it is currently subject to an administrative penalty referred to in Article 109(1) of the above-mentioned regulation.
- In compliance with article 107 of the abovementioned Regulation , and as far as the current grant award procedure is concerned, our organisation:
  g) is not subject to a conflict of interest;
  h) has not made false declarations in supplying the information required by the Commission as a condition of participation in the grant award procedure or does not fail to supply this information;
  i) is not in one of the situations of exclusion, referred to in the abovementioned points a) to f).

2- As an authorised representative to sign the grant agreement or to commit the abovementioned organisation, I also certify that our organisation:

- is committed to participate in the abovementioned project;
- has stable and sufficient sources of funding to maintain its activity throughout its participation in the abovementioned project and to provide any counterpart funding necessary;
- has or will have the necessary resources as and when needed to carry out its involvement in the abovementioned project.

3- As an authorised representative to sign the grant agreement or to commit the abovementioned organisation, I finally certify that all the information relating to our organisation set out in the different Grant Agreement Preparation Forms are complete, accurate and correct; and that the estimated costs meet the criteria for eligible costs for FP7 projects – as established by the ERC model grant agreement – are notably based on our usual accounting and management principles and practices, and reflect the costs expected to be incurred in carrying out the foreseen work described in Annex I (description of work).

4- Our organisation is fully aware that the Commission may impose administrative or financial penalties on legal entities who are guilty of misrepresentation in supplying the information required by the Commission as a condition of participation in the grant award procedure or fail to supply this information; have been declared to be in serious breach of their obligations under any contract/grant agreement covered by the budget of the Commission . Such penalties shall be proportionate to the importance of the contract/grant agreement and the seriousness of the misconduct, and may consist in their exclusion from the

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A2.6:
Data Protection & Coordination Role

Project number[1]	339446	Project acronym[2]	BIC	Host Institution number in this project[10]	1	Host institution short name[11]	Uniroma1

Signed only by the Host Organisation – Participant No. 1

Certified declaration on data protection by the Host Organisation

"All personal data contained and related to the Grant Agreement(such as names, addresses, CVs, etc.) will be processed in accordance with Regulation (EC) No. 45/2001 of the European Parliament and of the Council of 18 December 2000 on the protection of individuals with regard to the processing of personal data by the institutions and bodies of the European Union and on the free movement of such data (Official Journal L 8, 12.01.2001). Such data will be processed solely in connection with the implementation and follow-up of the Grant Agreement and the evaluation and impact assessment of European Union activities, including the use and dissemination of foreground, without prejudice to the possibility of passing the data to the bodies responsible for inspection and audit in accordance with European Union legislation and this Grant Agreement.

Principal Investigator, team members and beneficiaries/participants may, on written request, gain access to their personal data and correct any information that is inaccurate or incomplete. They should address any question regarding the processing of their personal data to the controller/s. They may lodge a complaint against the processing of their personal data with the European Data Protection Supervisor at any time.

For the purposes of this project, the Controller/s identified in Article 8.4 of the Grant Agreement shall be the contact/s for the Commission/ERC DIS (European Research Council Dedicated Implementation Structure).

Any sensitive information or material used as background or produced as foreground in this project is covered by a Security Aspect Letter (SAL)[39] which is provided. If sensitive information or material is found to be required at a later stage of the project, amendment to the grant agreement will be requested and a SAL will be provided.

I also certify that our organisation is committed to act as the (principal) beneficiary of this project."

Participant legal name[13]	UNIVERSITA DEGLI STUDI DI ROMA LA SAPIENZA		
Family name of authorised representative	Graziani	First Name(s)	Giorgio
Date	12/12/2013	Signature of the authorised representative to sign the grant agreement or to commit the organisation[38]	[signature]
Family name of alternative authorised representative		First Name(s)	
Date		Signature of the alternative authorised representative to sign the grant agreement or to commit the organisation[38]	

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FINANCIAL IDENTIFICATION

PRIVACY STATEMENT http://ec.europa.eu/budget/execution/ftiers_fr.htm

PROJECT NUMBER 339446 **PROJECT ACRONYM** BIC

ACCOUNT NAME

ACCOUNT NAME (1)	DIPARTIMENTO DI INGEGNERIA MECCANICA E AEROSPAZIALE
ADDRESS	Via Eudossiana 18
TOWN/CITY	Roma
POSTCODE	00184
COUNTRY	Italy

CONTACT (1)	Giuseppina Angeloni
TELEPHONE	+390644595936
FAX	+390644595250
E - MAIL	giuseppina.angeloni@uniroma1.it

BANK

BANK NAME	UNICREDIT SpA - Roma 153
BRANCH ADDRESS	P.le Aldo Moro 5
TOWN/CITY	Roma
POSTCODE	00185
COUNTRY	Italy
ACCOUNT NUMBER	
IBAN (2)	IT17P0200805227000400014557

REMARKS:

We certify that above information declared is complete and true.

BANK STAMP + SIGNATURE OF BANK REPRESENTATIVE (Both Obligatory) (3)	**DATE + SIGNATURE ACCOUNT HOLDER : (Obligatory)**

(1) The name or title under which the account has been opened and not the name of the authorized agent

(2) If the IBAN Code (International Bank account number) is applied in the country where your bank is situated

(3) It is preferable to attach a copy of recent bank statement, in which event the stamp of the bank and the signature of the bank's representative are not required. The signature of the account-holder is obligatory in all cases.

1. Project number

The project number has been assigned by the Commission as the unique identifier for your project, and it cannot be changed. The project number **should appear on each page of the grant agreement preparation documents** to prevent errors during its handling.

2. Project acronym

Use the project acronym as indicated in the submitted proposal. It cannot be changed, unless agreed during the negotiations. The same acronym **should appear on each page of the grant agreement preparation documents** to prevent errors during its handling.

3. Project title

Use the title (preferably no longer than 200 characters) as indicated in the submitted proposal. Minor corrections are possible if agreed during the preparation of the grant agreement.

4. Starting date

Unless a specific (fixed) starting date is duly justified and agreed upon during the preparation of the Grant Agreement, the ERC project will start on the first day of the month following the entry info force of the Grant Agreement (NB : entry into force = signature by the Commission). Please note that if a fixed starting date is used, you will be required to provide a detailed justification on a separate note.

5. Duration

Insert the duration of the project in full months.

6. Call (part) identifier

The Call (part) identifier is the reference number given in the call or part of the call you were addressing, as indicated in the publication of the call in the Official Journal of the European Union. You have to use the identifier given by the Commission in the letter inviting to prepare the grant agreement.

7. Activity code

Select the activity code from the drop-down menu.

8. Free keywords

Use the free keywords from your original proposal; changes and additions are possible.

9. Abstract

Use the abstract from your original proposal and amend to take account of the following: you should not use more than 2,000 characters, the abstract should, at a glance, provide the reader with a clear understanding of the objectives of the project and how the objectives will be achieved, as well as their relevance in the context of the objectives of the specific programme and the work programme. This summary will be used as the short description of the project for the public following signature of the grant agreement and in communications to the programme management committees and other interested parties. It must therefore be short and precise and should not contain confidential information. Please use plain typed text, avoiding formulae and other special characters.

10. Participant number

The host organisation of a project is always number one. Consequent numbers can be issued to other participants of this project.

11. Participant short name

The short name chosen by the participant. This should normally not be more than 20 characters and the same short name should be used for the participant in all documents relating to the project.

12. Participant identity code

To be completed when Unique Registration Facility will be operational.

13. Participant legal name

Official name of participant organisation (e.g. for host organisation or other participants). If applicable, name under which the participant is registered in the official trade registers.

14. Status of validation

If the status of validation of the participant is VALIDATED, this means the data provided in A2.1 has been validated by the Commission and this validated information is given in the A2.1 form.

Any entity engaged in an economic activity, irrespective of its legal form.

32. SME

SME means micro, small and medium sized enterprise within the meaning of Recommendation 2003/361/EC in the version of 6 May 2003 (see http://ec.europa.eu/enterprise/enterprise_policy/sme_definition/index_en.htm).

An enterprise is considered as an SME, taking into account its partner enterprises and/or linked enterprises (please see the above mentioned recommendation for an explanation of these notions and their impact on the definition), if it:

- employs fewer than 250 persons
- has an annual turnover not exceeding EUR 50 million, and/or
- an annual balance sheet total not exceeding EUR 43 million
- is autonomous

The headcount corresponds to the number of annual work units (AWU), i.e. the number of persons who worked full-time within the enterprise in question or on its behalf during the entire reference year under consideration. The work of persons who have not worked the full year, the work of those who have worked part-time, regardless of duration, and the work of seasonal workers are counted as fractions of AWU. The staff consists of:

- employees;
- persons working for the enterprise being subordinated to it and deemed to be employees under national law;
- owner-managers;
- is autonomous

partners engaging in a regular activity in the enterprise and benefiting from financial advantages from the enterprise.

ATTENTION: Apprentices or students engaged in vocational training with an apprenticeship or vocational training contract can not be included as staff. The duration of maternity or parental leaves is also not counted.

The data to apply to the financial amounts (e.g. turnover and balance sheet), as well as to the headcount of staff, are those relating to the latest approved accounting period and calculated on an annual basis. They are taken into account from the date of closure of the accounts. The amount selected for the turnover is calculated excluding value added tax (VAT) and other indirect taxes.

In the case of newly-established enterprises whose accounts have not yet been approved, the data to apply is to be derived from a bona fide estimate made in the course of the financial year. These organisations must insert "N/A" for the two questions relating to the duration and the closing date of their last approved accounting period.

33. Non-SME

An enterprise that is not an SME.

34. Title

Please choose one of the following: Prof.; Dr., Mr., Ms.

35. Gender

This information is required for statistical purposes. Please indicate with an F for female or an M for male as appropriate.

36. Position

Please indicate the position in your organisation e.g. Rector, President, Chief Executive Officer, Director etc.

37. Department/faculty/institute/laboratory name/...

Please indicate here the postal address for contact purposes.

38. Signature

The A2.4 and A2.5 forms needs to be signed by at least one of the authorised representatives indicated in the A2.3-form.

39. Security Aspect Letter

See Appendix 4 of the standard FP7 Negotiation Guidance Notes on http://cordis.europa.eu/fp7/find-doc_en.html.

40. Subcontracting

Costs include subcontracting and cost of resources made available by third parties which are not used on the premises of the beneficiary.

46. ICPC