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12 - Febbraio - 2017

### Componenti del Gruppo



#### Linee di Ricerca ERC - BIC

1. Microscale Wetting & Cavitation

M. Amabili (AR), A. Giacomello (RTD-A), E. Lisi (PhD), S. Marchio (PhD), S. Meloni (RTD-Collaborazioni: C. Valeriani (Universidad Complutense de Madrid)

2. Mesoscale Cavitation & Multiphase Flow Physics M. Gallo (PhD), F. Magaletti (AR), L. Marino (PA)

3. Macroscale Cavitation & Multiphase Flows

D. Pimponi (AR)

Collaborazioni: S. Chibbaro, S. Popinét (UPMC/Sorbonne)

4. Bubble Dynamics & Turbulent Transport

F. Battista (RTD-A), P. Gualtieri (RC), J.-P. Mollicone (AR)

5. Laser Induced Cavitation

D. Caprini (PhD), L. Marino (PA), A. Occhicone (PhD), G. Sinibaldi (AR) Collaborazioni: M. Chinappi (RTD-B Tor Vergata), F. Michelotti (PA SBAI), F. Pereira (INSEA

6. Cavitation in Biochips

D. Caprini (PhD), L. Marino (PA), C. Scognamiglio (PhD), G. Silvani (PhD), G. Sinibaldi (AR Collaborazioni: D. Durando (INRIM - Ultrasound Lab.), M. Kiani (Temple University), G. <u>Peruzzi (CLNS@IIT)</u>

#### Altre Linee di Ricerca

7. Experimental Microfluidics

D. Caprini (PhD), L. Marino (PA), C. Scognamiglio (PhD), G. Sinibaldi (AR) Collaborazioni: M. Chinappi (RTD-B Tor Vergata), X. Noblin (CNRS-LPMC), A. Nascetti (DI

8. After Implant Hemodynamics

G. Finesi (MS), F. Battista (RTD-A), P. Gualtieri (RC) Collaborazioni: M. Taurino (PO Medicina Clinica e Molecolare & AO S. Andrea)

*9. Microcombustors*F. Battista (RTD-A)Collaborazioni: S. Chibbaro (UPMC/Sorbonne)

10. Fundamental TurbulenceF. Battista (RTD-A), P. Gualtieri (RC), J.-P. Mollicone (AR)

Consistenza del gruppo: 1 PO, 1 PA, 1 RC, 3 RTD-A, 5 AR, 8 PhD S., 1 MS

Collaborazioni: Univ. Complutense Madrid, UPMS/Sorbonne Paris, Tor Ver



#### 35 Pubblicazioni 2013 -

Phys. Rev. Fluids (2s) J. Fluid Mech. (1s, 9)Phys. Rev. Let. (2) J. Phys: Cond. Mat. (1) J. Chem. Phys. (3)J. Mult. Phase Flows. (1) Soft Matter (1) New J. Phys. (1)Adv. Mat. Int. (1) Flow. Turb. Comb. (1) Europ. Phys. Let. (1) J. Phys.: Conf. S. (2) Phys. Fluids (2) Langmuir (2)Microfluidics & Nano. (2) Int. J. Heat Mass Tr. (1) Phys. Rev. E(1)I Phys Chem B(1)



## Fondi

- ERC Advanced Grant 2013: (BIC) Cavitation across scales Following
- Sapienza Awards 2014: Micro & Nanobubbles for Drug Delivery (53 k€)
- Grandi e Medie Attrezzature Sapienza: Cluster Menrva (120 k€)
- 5 PRACE Grants: CMC (2), P. Gualtieri (1), A. Giacomello (1, 2 year) (e
- Grandi e Medie Attrezzature Sapienza 2012: Sistema per Microscopia a Correla
- Fondi Gestione Microfluidic Lab (IIT-CLNS@Sapienza) (40 k€/year)

#### Strutture & Attrezzature

#### - Cluster Menrva

12 Nodi x 2 eptacore = 192 cores (CPU Intel Xeon E5-2650v2 2,6GHz, 64 Gb RAM) Switch Infiniband E6345, 40 Gb/s 12 Dischi 3 TB SATA, configurazione RAID 6 (30 TB)



- Microfluidic Lab IIT Center for Life Nanoscience@Sapienza



- Area Meccanica Applicata DIMA

# Sapienza Cluster: Menrva

- Grandi e Medie attrezzature: 1.2E+5 €
- More than 120 participants
  - Engineering, Physics
  - Mathematics, Chemistry
  - Biology, Pharmacy
  - Medicine
- 12 compute nodes: 384 cores
  - 32 cores per node
  - 64 Gb per node
  - 48Tb storage
  - Intel E5-2650 v2 @ 2.60GHz
  - InfiniBan connection
- Hosted at DIMA



**Menrva**: Etruscan Godness of war, art, wisdom and health

# Microscale Wetting & Cavitation

# Nanoscale wetting and cavitation

Origin of cavitation: homogeneous and heterogeneous nucleation



20 pm

People:

- Simone Meloni
- Alberto Giacomello
- Matteo Amabili
- Emanuele Lisi
- Antonio TintiSara Marchio

# Methods



INCREASING LENGTH  $\longrightarrow$ 

# Technological applications of superhydrophobic (submerged) surfaces



**Boiling heat transfer** 





Lotusan - the facade paint with the self-cleaning capacity of the lotus leaf.

Lotus-Effect

Wetting/dewetting of nanopillared submerged surfaces: micro vs macro

Simple fluid on a simple solid
 Both are LJ
 Solid-fluid

$$v(r) = 4\epsilon \left( \left(\frac{\sigma}{r}\right)^{12} - c \left(\frac{\sigma}{r}\right)^6 \right) \right)$$
  
$$\theta_Y \sim 110^\circ$$



Most probable dewetting path as a function of the density field

Not the usual observable vapor volume
Energetics

M. Amabili et al, submitted to Phys. Rev. Fluids

# Atomistic dewetting Mechanism and energetics

Sag transition



e-pinning transition



# **Robust Submerged Superhydrophibicity:** Salvinia molesta



Barthlott et al, Adv. Mat. 22, 2325 (2010)

# Model System

# piston $F_y$ Wh . 1 2. 19 A

# Combined chemistry model

Phobic interior



M. Amabili, A. Giacomello,\* S. Meloni, and C. M. Casciola

# Design principles for self-recovery superhydrophobic surfaces

Self-recovery

Minimal solid fraction



# Design principles of self-recovery surfaces for drag reduction



self-recovery

# Drag reduction

# Cavitation in nanoporous materials



 $\Phi$ 

## Rare event MD: cavitation in a nanopore



Physics of nanoconfined water (D=2 nm):

- cavitation at P=20 MPa
- intrusion at P=80 MPa
- hysteresis in intrusion/extrusion cycles

Applications of hydrophobic nanopores + water:

- energy storage: surface energy
- dampers: dissipation in intrusion/extrusion cycles

# Cavitation at the Mesoscale & Multiphase Flow Physics

Diffuse interface model for liquid-vapor phase transitions

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 & \text{Francesco Magaletti (DIMA)} \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) &= \nabla \cdot \mathbf{T} & \text{Luca Marino (DIMA)} \\ \frac{\partial \hat{e}}{\partial t} + \nabla \cdot (\mathbf{u}\hat{e}) &= \nabla \cdot (\mathbf{T} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}_e \end{aligned}$$
The free-energy functional  $F = \int_{\mathcal{D}} \hat{f} \, dV = \int_{\mathcal{D}} \left( \hat{f}_0(\rho, \theta) + \frac{\lambda}{2} |\nabla \rho|^2 \right) dV$   
leads to the constitutive equations:  
$$\mathbf{T} = \mu \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) + \eta \nabla \cdot \mathbf{u} \mathbf{I} + \\ -\lambda \nabla \rho \otimes \nabla \rho - \left[ p_0 + \frac{1}{2} \left( -\lambda + \rho \frac{\partial \lambda}{\partial \rho} \right) |\nabla \rho|^2 - \rho \nabla \cdot (\lambda \nabla \rho) \right] \mathbf{I} \\ \mathbf{q}_e = -k \nabla \theta + \lambda \rho \nabla \rho \nabla \cdot \mathbf{u} \end{aligned}$$

#### Collapse dynamics in free space



Density field (top) Pressure gradient (bottom)

(pressure gradient visualizes bubble interface and radiated shock)

- Strong overpressure prevents complete condensation (rebounds)
- A shock wave is emitted at rebound
- Strong thermal effects (sub-micron bubbles)
- Successive rebounds emit weaker and waker shocks



PRL 114, 064501 (2015)

PHYSICAL REVIEW LETTERS

week ending 13 FEBRUARY 2015

#### Shock Wave Formation in the Collapse of a Vapor Nanobubble

F. Magaletti, L. Marino, and C. M. Casciola\*

### A cartoon of collapse dynamics



#### Color legend

- Liquid phase
- Supercritical phase
- Vapour phase

- supercritical fluid (incondensable —> rebound)
- For insufficient compression vapour fully condensates





- Vapor bubble with in equilibrium with liquid (radius  $R_{eq}$ , center at  $z_0$
- Impinging shockwave intensity  $I = (p_2 p_1)/p_1$
- Simulations for different  $z_0$  and I





 $I = 400, \ z_0/R_{eq} = 2.2$ 



The axial flow after bubble collapse convects the re-expanding bu

#### Pressure

Temperature





- Pressure and temperature peaks at minimum bubble volume
- Pressure peak at the wall
- Huge wall pressure peak when the bubble gets close to the wall (second collapse)

Fluctuating Hydrodynamics & Cavitation

# Fluctuating Hydrodynamics (Lifshitz, Landau, Uhlembeck, Onsager) • Entropy Functional and Fluctuations $\Delta S = S - S_0 = \Delta S \left[\delta \rho, \delta \mathbf{v}, \delta \theta\right] = \int_V s \left(\mathbf{x}, t\right) - s_0 \, dV$ $P_{eq} \left[\Delta\right] = \frac{1}{Z} e^{\frac{\Delta S}{k_B}} \simeq \frac{1}{Z_0} e^{-\frac{1}{2k_B} \int_V \Delta^T \mathbf{H} \Delta \, dV} \qquad \Delta = (\delta \rho, \delta \mathbf{v}, \delta \theta)$

• Functional Langevin Equation

$$\partial_t \Delta = \mathbf{M} \cdot \frac{\delta \Delta S_0}{\delta \Delta} + \mathbf{f} \qquad \mathbf{f} = \mathbf{K} W$$

$$\frac{\delta \Delta S_0}{\delta \Delta} = -\mathbf{H} \cdot \mathbf{\Delta} \qquad \mathbf{M} = \mathbf{L} \mathbf{H}^{-1}$$

$$\mathbf{L} = \begin{pmatrix} 0 & -\rho \partial_x & 0\\ -\frac{c_T^2}{\rho_0} \partial_x & \frac{\mu}{\rho_0} \partial_{xx} & -\frac{1}{\rho_0} \partial_\theta p \partial_x\\ 0 & -\frac{\theta_0}{\rho_0 c_v} \partial_\theta p \partial_x & \frac{k}{\rho_0 c_v} \partial_{xx} \end{pmatrix} \qquad \mathbf{K} = \begin{pmatrix} 0 & 0 & 0\\ 0 & \frac{\sigma_v}{\rho_0} & 0\\ 0 & 0 & -\frac{\sigma_\theta}{\rho_0 c_v} \end{pmatrix}$$

• Fluctuation Dissipation  $\sigma_v = \sqrt{2\mu\theta_0}\partial_x$  $\mathbf{Q} = k_B \left( \mathbf{M} + \mathbf{M}^{\dagger} \right) \delta \left( \hat{x} - \tilde{x} \right) \qquad \sigma_{\theta} = \sqrt{2k_0\theta_0^2}\partial_x$ 

#### Vapour Nucleation & Fluctuating Hydrodynamics



# Bubble Dynamics & Turbulent Transport

# Micro-Macro-Micro



- Microscopic inception: MD
- Macroscopic transport: turbulence
  - micro-bubbles radius dynamics (Rayleigh-Plesset)
  - turbulence modulation (ERPP)
  - large bubbles (VoF)
- Microscopic collapse: PF

# Micro-bubble dynamics

Newtons' law



Stokes Number

$$\tau_p = \left(\frac{\rho_p}{\rho_f} + \frac{1}{2}\right) \frac{d_p^2}{18\nu} \Rightarrow \frac{St_\eta}{\tau_\eta} = \frac{\tau_p}{\tau_\eta}$$

$$eta = rac{3}{2\left(rac{
ho_p}{
ho_f}+rac{1}{2}
ight)}$$

#### clustering

$$abla \cdot \mathbf{v} = au_p(eta - 1) \left(S^2 - \Omega^2\right) < 0$$

- bubbles  $\beta = 3 \Rightarrow \Omega > S$
- particles  $\beta = 0 \Rightarrow \Omega < S$

S =strain rate;  $\Omega =$ rotation rate
### Bubbles in the Box



Iso-surfaces of the "D" invariant: coherent vortical structures & instantaneous bubble position

### Bubble radius dynamics: Rayleigh-Plesset

$$R\frac{d^2R}{dt^2} + \frac{3}{2}\left(\frac{dR}{dt}\right)^2 + \frac{4}{Re}\frac{1}{R}\frac{dR}{dt} + \frac{2}{We}\frac{1}{R} = p_b(t) - p_f[\mathbf{x}_b(t)]$$

Gas bubble: Isentropic  $p_b(t)V_b^{\gamma}(t) = p_{b,0}V_{b,0}^{\gamma}$ 

Turbulent pressure signal  $p_f[\mathbf{x}_b(t)] = p_0 + p'[\mathbf{x}_b(t)]$   $We = \frac{\text{inertia}}{\text{surface tension}}$ 



### Bubble radius dynamics: Rayleigh-Plesset

$$R\frac{d^2R}{dt^2} + \frac{3}{2}\left(\frac{dR}{dt}\right)^2 + \frac{4}{Re}\frac{1}{R}\frac{dR}{dt} + \frac{2}{We}\frac{1}{R} = p_b(t) - p_f[\mathbf{x}_b(t)]$$

Gas bubble: Isentropic  $p_b(t)V_b^{\gamma}(t) = p_{b,0}V_{b,0}^{\gamma}$ 

Turbulent pressure signal  $p_f[\mathbf{x}_b(t)] = p_0 + p'[\mathbf{x}_b(t)]$   $We = \frac{\text{inertia}}{\text{surface tension}}$ 



## Can a bubble blow-up?



- Intermittent pressure bursts
- Intrinsic RP time-scale to be correlated with
  - pressure correlation time-scale
  - time spent in negative pressure regions

#### Micro-Bubble Transport in Turbulence





Microfluidic Lab



- Micro-PIV
- Fluorescence Confocal Microscopy
- High Speed Imaging
- Fiber Optic Hydrophone
- Micro-fabrication
- Cell-culture







- Micro-PIV
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- Micro-PIV
- Fluorescence Confocal Microscope
- High Speed Imaging
- Fiber Optic
  Hydrophone
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Confocal microscope (Olympus iX73 FluoView1220) operated in epi-fluorescence

Evolve 512 Delta EMCCD camera





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### Photron Mini UX1000



- CMOS sensor
- $10 \ \mu m \ x \ 10 \ \mu m \ pixel size$
- Resolution 1280 x 1024
- 4000 fps @ full frame
- 800.000 fps @ 1D



- Micro-PIV
- Fluorescence Confocal Microscopy
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- Cell-culture



#### SBAI – La Sapienza



- Micro-PIV
- Fluorescence Confocal Microscopy
- High Speed Imaging
- Fiber Optic Hydrophone
- Micro-fabrication
- Cell-culture

## Lithography Mask UV PROJECTOR UV light Photoresist





DIET – La Sapienza





- Micro-PIV
- Fluorescence Confocal Microscopy
- High Speed Imaging
- Fiber Optic Hydrophone
- Micro-fabrication
- Cell-culture





Cavitation in Biochips



**Department of Mechanical and Aerospace Engineering** 



# **Cavitation enhanced drug delivery**

Giulia Silvani (DIMA - IIT)

- Chiara Scognamiglio (DIMA LPMC)
- Davide Caprini (DIMA)
- Giorgia Sinibaldi (DIMA)
- Luca Marino (DIMA)

Mauro Chinappi (Torvergata)





**Giovanna Peruzzi** 



## Cavitation enhanced drug delivery

### Blood vessel on a chip



Deosarkar et al., PLOS ONE 2015

#### Permeability measurements



## Cavitation enhanced drug delivery Unique features of the device





- Realistic sizes
- Correct perfusion rate
- Correct physiological shear stress intensity
- Ability to reproduce the biochemical interactions between tumor and endothelium



Hao-Li Liu et al., Theranostics 2014

## Cavitation enhanced drug delivery

#### Ultrasounds chain



Experimental Microfluidics



**Department of Mechanical and Aerospace Engineering** 



# **Experimental Microfluidics**

- Davide Caprini (DIMA)
- Chiara Scognamiglio (DIMA LPMC)
- Giorgia Sinibaldi (DIMA)
- Luca Marino (DIMA)
- Mauro Chinappi (Torvergata)





DIET - Dipartimento di Ingegneria Elettrica e Telecomunicazioni

Prof. A. Nascetti





## Bubbles in micro-devices MicroPIV + high speed imaging













## Cavitation confined in Micro-system



Biomimetic device fabrication





## Bubbles acoustic signature





20 µm walls





Laser Induced Cavitation



**Department of Mechanical and Aerospace Engineering** 



## Laser Induced Cavitation Bubble

- Giorgia Sinibaldi (DIMA)
- Davide Caprini (DIMA)
- Agostino Occhicone (DIMA –SBAI)
- Luca Marino (DIMA)
- Mauro Chinappi (Torvergata)







SBAI - Dipartimento di Scienze di Base Applicate all'Ingegneria

Prof. F. Michelotti





## Bubble dynamics



(Interframing time 12,5  $\mu$ s)

			_		
80000 fps +0.1250 ms	1280 x 56 Date : 2016/12/19	frame : 10 Time : 15:42	80000 fps +0.3625 ms	1280 x 56 Date : 2016/12/19	frame : 29 Time : 15:42
80000 fps +0.1375 ms	1280 x 56 Date : 2016/12/19	frame : 11 Time : 15:42	80000 fps +0.3750 ms	1280 x 56 Date : 2016/12/19	frame : 30 Time : 15:42
80000 fps +0.1500 ms	1280 x 56 Date : 2016/12/19	frame : 12 Time : 15:42	80000 fps +0.3875 ms	1280 x 56 Date : 2016/12/19	frame : 31 Time : 15:42
80000 fee	1200 56	frame 12	90000 fee	1200 - 56	firme - 22
+0.1625 ms	Date : 2016/12/19	Time : 15:42	+0.4000 ms	Date : 2016/12/19	Time : 15.42
80000 fps	1280 x 56	frame: 14	80000 fps	1280 x 56	frame : 33
+0.1750 ms	Date : 2016/12/19	Time : 15:42	+0.4125 ms	Date : 2016/12/19	Time : 15:42
80000 fps +0.1875 ms	1280 x 56 Date : 2016/12/19	frame : 15 Time : 15:42	80000 tps +0.4250 ms	1280 x 56 Date : 2016/12/19	frame : 34 Time : 15:42
80000 tps +0.2000 ms	1280 x 56 Date : 2016/12/19	frame : 16 Time : 15:42	80000 tps +0.4375 ms	1280 x 56 Date : 2016/12/19	frame : 35 Time : 15:42
80000 fps +0.2125 ms	1280 x 56 Date : 2016/12/19	frame : 17 Time : 15:42	80000 fps +0.4500 ms	1280 x 56 Date : 2016/12/19	frame : 36 Time : 15:42
80000 tps +0.2250 ms	1280 x 56 Date : 2016/12/19	frame : 18 Time : 15:42	80000 fps +0.4625 ms	1280 x 56 Date : 2016/12/19	frame : 37 Time : 15:42
80000 fps +0.2375 ms	1280 x 56 Date : 2016/12/19	frame : 19 Time : 15:42	80000 fps +0.4750 ms	1280 x 56 Date : 2016/12/19	frame : 38 Time : 15.42
80000 fps +0.2500 ms	1280 x 56 Date: 2016/12/19	frame : 20 Time : 15:42	80000 fps +0.4875 ms	1280 x 56 Date : 2016/12/19	frame : 39 Time : 15:42
80000 tps +0.2625 ms	1280 x 56 Date : 2016/12/19	frame: 21 Time: 15:42	80000 fps +0.5000 ms	1280 x 56 Date : 2016/12/19	frame : 40 Time : 15:42
				1000 50	
80000 fps +0.2750 ms	1280 x 56 Date : 2016/12/19	frame : 22 Time : 15:42	80000 tps +0.5125 ms	1280 x 56 Date : 2016/12/19	frame: 41 Time: 15:42
80000 fps +0.2875 ms	1280 x 56 Date : 2016/12/19	frame : 23 Time : 15:42	80000 fps +0.5250 ms	1280 x 56 Date : 2016/12/19	frame : 42 Time : 15.42
80000 tps +0.3000 ms	1280 x 56 Date : 2016/12/19	frame : 24 Time : 15:42	80000 tps +0.5375 ms	1280 x 56 Date : 2016/12/19	frame : 43 Time : 15:42
20200 1	1290 - 50	frame OF	00000	1000 - 50	
+0.3125 ms	Date : 2016/12/19	Time: 15:42	+0.5500 ms	Date : 2016/12/19	Time : 15:42
20200	1000.00	frame AA	00000	1000 50	
+0.3250 ms	Date : 2016/12/19	Time: 15:42	80000 tps +0.5625 ms	1280 x 56 Date : 2016/12/19	frame: 45 Time: 15:42
80000 foe	1280 x 56	frame : 27	80000 foe	1280 x 56	frame : 46
+0.3375 ms	Date : 2016/12/19	Time : 15:42	+0.5750 ms	Date : 2016/12/19	Time : 15.42
	)				
80000 fps +0.3500 ms	1280 x 56 Date : 2016/12/19	frame : 28 Time : 15:42	80000 fps +0.5875 ms	1280 x 56 Date : 2016/12/19	frame : 47 Time : 15:42

@SAPIENZ.



## "Spherical" rebound







## Plasma Analysis Multiple plasma



Three plasmas - one bubble



laser





534 μm

(same laser energy)



#### Three plasmas - three bubbles



## Hydrophone

Breakdown shock wave emission















Tagawa et al 2016

After Implant Hemodynamics



## After Implant Hemodynamics **Z**Endologix







Giorgio Finesi (MS DIMA/DMCM) Francesco Battista (DIMA) Paolo Gualtieri (DIMA)



DMCM - Dipartimento di Medicina Clinica e Molecolare

M. Taurino



Microcombustors


## Microcombustors

Francesco Battista (DIMA) Gianmatteo Carapellotti (MS DIMA) Matteo Hakimi (MS DIMA/UPMS)



а **Opposite propagating flames** U shaped flame с Q Channel 2 -UH **Channel 1** +U U  $x_{f1} - L \rightarrow x_{f2}$ 

b

CNRS - Laboratoire de Combustion et

Systemes Reactifs Gueening. anglet Fuel/air Test section: Flame  $U_a$  (cm/s) xternal heat source (e.g., H<sub>2</sub>/air burner)

Lithium ion batteries E = 0.2 kWh/kg\* micro combustors E=10 kWh/kg \*



Fundamental Turbulence



## Fundamental Turbulence



Francesco Battista (DIMA)Paolo Gualtieri (DIMA)Jean-Paul Mollicone (DIMA)

Previous collaborations:

E. De Angelis, A. Cimarelli, I. Marusich,

E. Longmire, X. Jimenez