

Local Organiser:



Grant Holder:



**SimInhale**  
COST ACTION  
MP1404



## SIMINHALE COST ACTION MP1404

Simulation and pharmaceutical technologies for advanced patient-tailored inhaled medicines

### WORKSHOP

## “Pulmonary Drug Delivery: Computational Fluid Particle Dynamics and Emerging Functional Imaging Technologies”

Prague, October 18-19, 2016

Organised by:

UCY-CompSci Lab, University of Cyprus (Prof. Stavros Kassinos, Grant Holder)  
WG3 Leaders Prof. Martin Sommerfeld and Prof. Alessio Alexiadis  
WG4 Leaders Dr. Jan de Backer and Dr. Kaye Morgan

Hosted by:

Institute of Chemical Process Fundamentals of the Czech Academy of Sciences, Czech Republic, Dr. Vladimír Zdimal  
Fakulta strojního inženýrství - Brno University of Technology, Dr. Miroslav Jicha

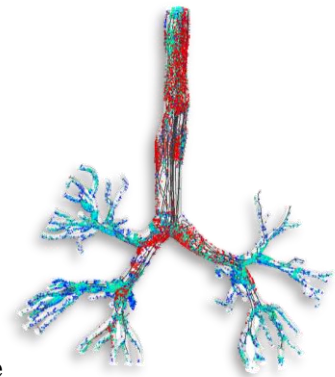
### *Workshop overview and objectives*

This will be an intensive two-day workshop on the current state of the art on Pulmonary Drug Delivery from the perspective of Computational Fluid Particle Dynamics (CFPD) and Emerging Functional Imaging Technologies. The workshop features an interesting mix of talks and features lecturers from the academic and research communities, the industry and the medical professions.

Through the workshop the following aspects will be tackled:

- State of the art in human airways model construction
- Biodistribution of inhaled agents in health and disease
- Inhaler devices design and optimization issues
- Quantifying regional deposition via CFPD and lung imaging

Workshop participants can participate in the CFPD computation of a selected benchmark case. Results and comparison will be presented at the workshop. If you are interested to join this effort please contact Prof. Stavros Kassinos ([kassinos@ucy.ac.cy](mailto:kassinos@ucy.ac.cy)) or Prof. Martin Sommerfeld ([martin.sommerfeld@iw.uni-halle.de](mailto:martin.sommerfeld@iw.uni-halle.de))





## Keynote Speakers



**Professor Ching-Long Lin**  
*The University of Iowa, USA*  
*Computational Physics Laboratory*  
<http://user.engineering.uiowa.edu/~ching/>



**Professor Yu Feng (USA)**  
*Oklahoma State University,*  
*Computational Biofluidics and Biomechanics Lab*  
<http://www.cbbl-okstate.com>

## Confirmed Speakers

(in alphabetical order)

- Dr. Alessio Alexiadis, University of Birmingham, United Kingdom
- Dr. Per Backman, Mylan Pharma UK Ltd., United Kingdom
- Dr. Joy Conway, University of Southampton. United Kingdom
- Dr. Yannick Crémillieux, Université de Bordeaux, France
- Dr. Sandra Cvijić, University of Belgrade, Serbia
- Dr. Marcel Filoche, Ecole Polytechnique, CNRS, France
- Dr. Stavros Kassinos, University of Cyprus, Cyprus
- Pantelis Koullapis, University of Cyprus, Cyprus
- Mary Devlin Capizzi, International Pharmaceutical Aerosol Consortium on Regulation & Science (IPAC-RS)
- Dr. František Lízal, Brno University of Technology, Czech Republic
- Dr. Oriol Lehmkuhl, Catalonia to Barcelona Supercomputer Center, Spain
- Dr. François Lux - Institut Lumière Matière, France
- Dr. Kaye Morgan, Technische Universität München, Germany
- Dr. Denise Morris, Simulation Plus Inc., USA
- Dr. Martin Sommerfeld, Martin Luther University Halle-Wittenberg, Germany
- Dr. Josue Sznitman, Technion - Israel Institute of Technology, Israel
- Dr. Sylvia Verbanck, Oncologisch Centrum UZ Brussel, Belgium
- Dr. Irene Vignon-Clementel, INRIA de Paris & Sorbonne Universités, France
- Dr. Herbert Wachtel, Boehringer Ingelheim, Germany

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## Workshop Agenda

Tuesday October 18, 2016

Time	Description
8:30	Registration
9:00	Welcome by Local Organizer
9:15	Welcome by MP1404 Chair
9:30	<b>Keynote Speaker: Prof. Ching-Long Lin, University of Iowa (USA)</b> A Multi-scale imaging-based statistics-guided predictive lung model with potential application to drug delivery
10:15	TBA <b>Mary Devlin Capizzi, IPAC-RS Secretariat</b>
10:45	<i>Coffee Break</i>
11:15	Orally inhaled product properties governing deposition and exposure in man – case for a standardised approach to deposition modelling? <b>Dr. Per Backman, Mylan Pharma UK Ltd. (United Kingdom)</b>
11:45	Unravelling the fate of inhaled aerosols in the pulmonary depths in silico and in vitro <b>Dr. Josue Sznitman, Technion - Israel Institute of Technology, Israel</b>
12:15	Surfactant delivery in the lung airway systems: new insights <b>Dr. Marcel Filoche, Ecole Polytechnique, CNRS, France</b>
13:00	<i>Lunch</i>
14:30	Deposition and absorption of inhaled drugs: Possibilities and limitations of physiologically-based in silico modelling <b>Dr. Sandra Cvijić, University of Belgrade, Serbia</b>
15:00	High speed in vivo x-ray phase contrast imaging for respiratory treatment development <b>Dr. Kaye Morgan, Technische Universität München, Germany</b>
15:30	Respiratory Imaging <b>Dr. Joy Conway, University of Southampton. United Kingdom</b>
16:00	<i>Coffee Break</i>
16:30	Multi-D models for respiration and aerosol in health and disease <b>Dr. Irene Vignon-Clementel, INRIA de Paris &amp; Sorbonne Universités, France</b>
17:00	Modelling of mass transfer in ciliated boundary layers <b>Dr. Alessio Alexiadis, University of Birmingham, United Kingdom</b>
17:30	Applications of physiologically based pharmacokinetic (PBPK) modeling in pulmonary drug delivery <b>Dr. Denise Morris, Simulation Plus Inc., USA</b>
18:00	End of Day 1

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Wednesday October 19, 2016

Time	Description
9:00	Registration
9:15	Overview of Day 2 by MPI1404 Chair
9:30	<b>Keynote Speaker: Yu Feng, Oklahoma State University, USA</b> Advanced computational fluid-particle dynamics (CF-PD) models for unconventional inhaled aerosols in human upper airways
10:15	<i>Coffee Break</i>
10:45	Comparison of two inhaler devices including wall collision detachment <b>Dr. Martin Sommerfeld, Martin Luther University Halle-Wittenberg, Germany</b>
11:15	Applying ANSYS Fluent in the analysis of dry powder inhalers <b>Dr. Herbert Wachtel, Boehringer Ingelheim, Germany</b>
11:45	Using standardized mouth-throat geometries for the in silico assessment of regional deposition in the conducting airways <b>Dr. Stavros Kassinos, University of Cyprus, Cyprus</b>
12:15	Biodistribution imaging of inhaled contrast agents and nanoparticles using MRI <b>Dr. Yannick Crémillieux, Université de Bordeaux, France</b>
13:00	<i>Lunch</i>
14:30	Inhaled aerosol distribution in human airways: A scintigraphy-guided study in a 3D printed model <b>Dr. Sylvia Verbanck, Oncologisch Centrum UZ Brussel, Belgium</b>
15:00	Ultrasmall gadolinium based nanoparticles for image guided radiotherapy of lung tumors <b>Dr. François Lux - Institut Lumière Matière, France</b>
15:30	Integrated solutions for the direct numerical simulation of airflow and particle deposition in the respiratory system <b>Dr. Oriol Lehmkuhl, Catalonia to Barcelona Supercomputer Center, Spain</b>
16:00	<i>Coffee Break</i>
16:30	The lung model test case - presentation of the available experimental data <b>Dr. František Lízal, Brno University of Technology, Czech Republic</b>
17:00	The lung model test case – comparison of simulations results from the collaborative work of WG3 members <b>Mr. Pantelis Koullapis, University of Cyprus, Cyprus</b>
17:30	<b>Discussion and Farewell</b>

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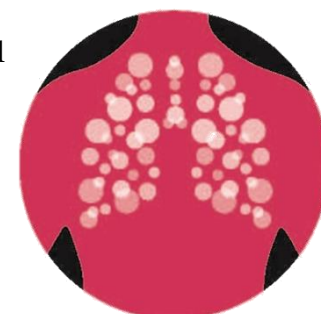
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## *SimInhale COST Action MP1404*

As a result of the culmination of several scientific and technological developments, we are on the verge of technological breakthroughs in the field of inhaled medicines that will revolutionize the treatment of many acute or chronic respiratory and systemic illnesses. However, knowledge in the field is vertically fragmented and compartmentalized in disciplines. As a result, current developments are not necessarily synergistic and supportive of each other. The prospect of patient-tailored inhaled medicines necessitates a much closer coordination of research and development activities.

The primary objective of Siminhale is to develop create and maintain a pan-European multidisciplinary scientific network that will coordinate and enhance research and development (R&D) in the field of inhaled medicines with the aim to accelerate the development of a new generation of effective and safe inhaled medicines.



Siminhale aims to create a pan-European network of experts in order to: i) advance particle designs for improved deposition and interaction with lung tissue, ii) promote realistic computer simulations of particle aerosolization, delivery and deposition, iii) promote patient-tailored inhaled medicines, iv) promote integration of device and formulation design, and v) promote critical assessment of toxicity issues and related risks. Making a new generation of advanced inhaled pharmaceuticals available to patients in a shorter period of time will have enormous social benefits.

Learn more on the Action on: [www.siminhale-cost.eu](http://www.siminhale-cost.eu)

LinkedIn: <https://www.linkedin.com/groups/8421105>

Facebook: <https://www.facebook.com/siminhale/>

For more information please contact Mr. Toumazis Toumazi [toumazis@ucy.ac.cy](mailto:toumazis@ucy.ac.cy)

“The COST Action MP1404 – SimInhale is supported by COST (European Cooperation in Science and Technology)”.

COST (European Cooperation in Science and Technology) is a pan-European intergovernmental framework. Its mission is to enable break-through scientific and technological developments leading to new concepts and products and thereby contribute to strengthening Europe’s research and innovation capacities. It allows researchers, engineers and scholars to jointly develop their own ideas and take new initiatives across all fields of science and technology, while promoting multi- and interdisciplinary approaches. COST aims at fostering a better integration of less research intensive countries to the knowledge hubs of the European Research Area. The COST Association, an International not-for-profit Association under Belgian Law, integrates all management, governing and administrative functions necessary for the operation of the framework. The COST Association has currently 36 Member Countries. [www.cost.eu](http://www.cost.eu)