BUSINESS DECISION SUPPORT SYSTEM (BDSS) IN FORMULATIONS AND COMPUTATIONAL ENGINEERING

17th - 18th February 2021

BDSS-ONLINE WORKSHOP

One of the effects of COVID, by limiting access to experimental data measured physically, has been to dramatically emphasise the value of being able to design products and select new ingredients in-silico. So minimising the number of physical experiments that need to be performed in the lab. The FORCE consortium is a pan-European project of 10 expert partners with the objective to develop an integrated Business Decision Support System (BDSS) based on open standards for industries engaged in formulating chemical ingredients.

This workshop will present the scientific achievements of the project along with the tools that have been developed so that scientists who are not expert modellers can utilise these new capabilities in a simple to use environment.

This will cover, the capabilities developed for partners within Unilever for new surfactants, DOW and Megara.

17th of February 2021		**All times are in Central European time zone (CET)**
CET		
10:30	Materials Modelling under Horizon Europe	Javier Sanfélix, European Commission
10:45	Force: an overview of the EU funded project on Formulations and computational engineering	Torsten Kraft, Fraunhofer IWM
11:15	Multi criteria optimisation within the BDSS	Peter Klein, Fraunhofer ITWM
11:45	Data management within FORCE	Davide Di Stefano, ANSYS
12:00	Introduction to SimPhoNy (ontology-based framework for interoperability between 3rd-party software tools)	Matthias Büschelberger, Fraunhofer IWM
12:15	BDSS Workflow Manager demo	Frank Longford, Enthought
12:30	**Lunch break**	

This Workshop is part of a project that has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement №721027.

13:30	Overview of Unilever's example for surfactant selection	Ian Stott, Unilever
13:45	Performing multiscale simulations of morphology and rheology of surfactant micelles	Vlasis Mavrantzas, Stavros Peroukidis, Terpsichori (Chara) Alexiou, University of Patras
14:45	Demonstration of Unilever's use case using the workflow manager	Frank Longford, Enthought
15:15	End of day 1	

18th of February 2021

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CET		
10:30	Overview of technical challenge for thermal insulation for DOW	Jerome Claracq, Tom Verbrugge, DOW
10:45	Fundamentals of foam moulding of refrigerator cabinets	Jerome Claracq, Terpsichori (Chara) Alexiou, DOW, University of Patras
11:15	Demonstration of DOW's use case	Matthias Büschelberger, Fraunhofer IWM
12:15	**Lunch break**	
13:15	Overview of technical challenge for modelling polyurethane resins' polymerisation reactions for Megara Resins	Poppy Krassa, MEGARA
13:30	Knowledge based inference modelling	n.n. IBM
14:00	Demonstration of Megara's use case	Giovanni Borzi Michele Dolfi, Enginsoft, IBM
14:30	Data management beyond FORCE	Davide Di Stefano, ANSYS
14:45	Extending the BDSS to new use cases	Frank Longford, Enthought
15:45	End of day 2	