Abstract of our keynote speaker Marc Geers

Multiscale mechanics of solids: microfluctuations matter!
The bottom-up design of advanced materials with unprecedented mechanical properties is a grand challenge, requiring reliable multiscale methods. The mechanical performance of engineering materials at the large scale often reveals particular emergent properties that originate from the complexity at the underlying fine scale level. Relating and predicting the macroscopic emergent behavior is a non-trivial task, for which classical homogenization methods may fall short. This presentation addresses this multi-scale challenge, whereby the microfluctuation fields at the fine scale are key in understanding and solving the problem. Two problems are addressed to illustrate the problem and potential solutions: (1) multiscale modelling of acoustic metamaterials, which are tailored to attenuate sound wave propagation for certain frequencies, (2) the multi-scale behaviour of delaminating cohesive interfaces of polymer-metal laminates, as used for stretchable electronics applications.

Abstract of our keynote speaker Patrick Perré

Coupled heat and mass transfer in porous media: upscaling, downscaling and multiscale modelling
This talk is devoted to multiscale approaches of coupled transfer in porous media, with particular attention to configurations leading to the failure of the assumption of local thermodynamic equilibrium. Upscaling methods, such as homogenization or volume averaging, allowed a well-established set of macroscopic equations to be obtained. This approach is powerful but needs to be supplied by relevant effective parameters. Nowadays, thanks to the spectacular progresses in 3D imaging and computational tools, these effective parameters can be obtained by 3D calculations on real pore morphologies. A recent example will be presented to predict properties of bio-based building materials. The remaining part of the talk will be devoted to configurations generating the absence of local thermodynamic equilibrium. Such situations, arising more often than expected, require a comprehensive multiscale approach. In one way or another, the local history of the product must be embedded in the formulation. Three approaches will be discussed here: (1) the concept of distributed micromodels, with various assumptions regarding the coupling between scales, (2) the transfer of all the information at the micro scale (downscaling), (3) the transfer of all the information at the macroscopic level, in which the concept of internal variables allows the history of the microscopic field to be transferred at the macroscopic level.
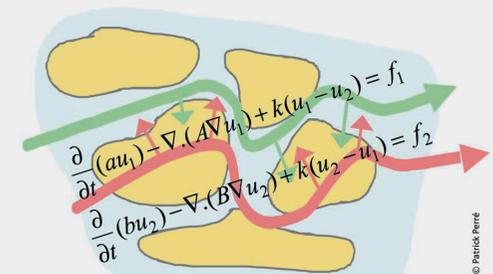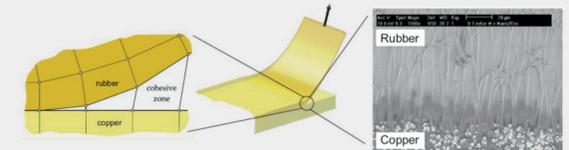
GENERAL INFORMATION

Location	Empa, Dübendorf Überlandstrasse 129 AKADEMIE
Cost	The event is sponsored by Empa and free of charge for the participants.
Registration	www.empa-akademie.ch/multiscale
Deadline	May 26, 2017
Contact	Empa **Dr Thijs Defraeye** Phone +41 58 765 47 90 thijs.defraeye@empa.ch www.empa.ch
How to get here	Please do use public transport. There is only very limited parking available.
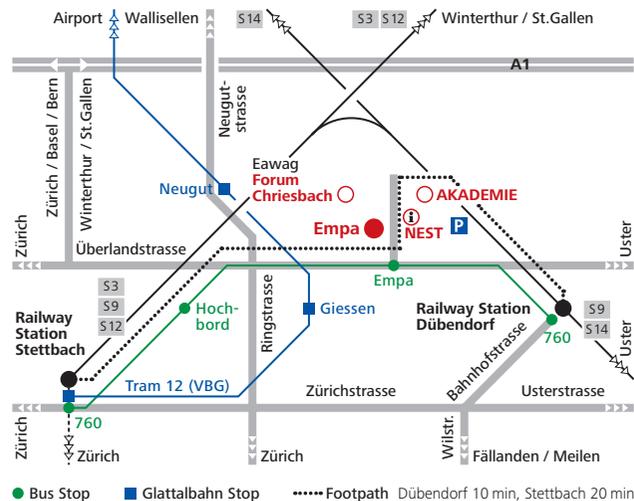
Empa Akademie

TOPICAL DAY

High-performance multiscale modelling IV

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$$\frac{\partial}{\partial t}(au_1) - \nabla.(A\nabla u_1) + k(u_1 - u_2) = f_1$$
$$\frac{\partial}{\partial t}(bu_2) - \nabla.(B\nabla u_2) + k(u_2 - u_1) = f_2$$

Empa, Dübendorf, Überlandstrasse 129
Tuesday, May 30, 2017, from 9:00 to 16:00

Online registration:
www.empa-akademie.ch/multiscale

TOPIC

Advanced simulations at nano- to environmental scales and linking of multiple scales, including electronic structure calculations, molecular dynamics, discrete element modelling, Lattice Boltzmann methods, continuum hygro-thermo-mechanical FEM and environmental computational fluid dynamics.

TARGET AUDIENCE

Scientists, PhDs and postdocs working with advanced computational models at different scales.

OBJECTIVES

This series of Topical Days offers a platform to experts in high-performance multiscale modelling on the latest developments and for sharing experiences. The focus is on solving computationally demanding problems in physics, chemistry, material science and engineering, ranging from nano- to environmental scale. Another point of interest is how to couple such simulations at different scales in an efficient and accurate way.

These Topical Days particularly aim to bring together the community at Empa and to link people with different backgrounds and skills.

For this fourth Topical Day, two keynote speakers are invited to share their latest research: **Prof. Marc Geers** (Eindhoven University of Technology, The Netherlands) and **Prof. Patrick Perré** (Université Paris-Saclay, France). For the remainder of the day, several Empa scientists will present examples of their modelling work. In addition, **Dr Falk Wittel** will present his recent activities at the Computational Physics for Engineering Materials group of the Institute for Building Materials of ETH Zürich. The progress regarding a center of competence at Empa is also discussed.

PROGRAM

8:30   Welcome Coffee, Registration

9:00   Opening remarks
Dr Thijs Defraeye

9:15   Multiscale mechanics of solids: microfluctuations matter!
Prof. Marc Geers,
Eindhoven University of Technology, The Netherlands

10:30   Coffee break

11:00   Examples and current work from colleagues at Empa

Virtual cold chain method to model the thermal behavior and quality evolution of packaged fresh fruit
Dr Wentao Wu, Multiscale Studies in Building Physics

Numerical modeling of shape memory effect of an iron-based SMA embedded in concrete
Dr Moslem Shahverdi, Structural Engineering

Structure-borne sound radiation modelling for railway rolling noise
Gwenael Hannema, Acoustics / Noise Control

11:45   Competence Center and cluster at Empa
Dr Thijs Defraeye / Dr Daniele Passerone

12:00   Lunch

13:15   Coupled heat and mass transfer in porous media: upscaling, downscaling and multiscale modelling
Prof. Patrick Perré, Université Paris-Saclay, France

14:30   Examples and current work from colleagues at Empa

An integrative model for the filtration efficiencies of airborne particles in realistic tests
Panagiota Sachinidou, Advanced Analytical Technologies

Modelling airflow and radiation through vegetation with a porous medium approach using OpenFOAM
Lento Manickathan, Multiscale Studies in Building Physics

15:00   Coffee break

15:30   Failure in wet granular matter
Dr Falk Wittel, ETH Zürich, Switzerland

16:00   Closing