Topical Days

Topical Days are an integral part of Empa's permanent education program for scientific and technical staff. The topics cover central aspects of research relevant for Empa and are intended to be of interest to many if not most Empa staff.

Typical topics cover

- Measurement Uncertainty
- Vacuum Technology
- Analytical Technologies
- Imaging Techniques

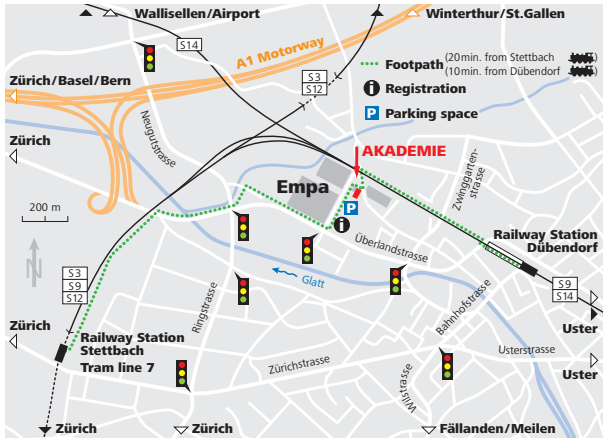
and many more.

Two to three Topical Days are planned each year.

We are always interested in new topics.

Please feel free to contact anne.satir@empa.ch
if you have any suggestions.

Directions



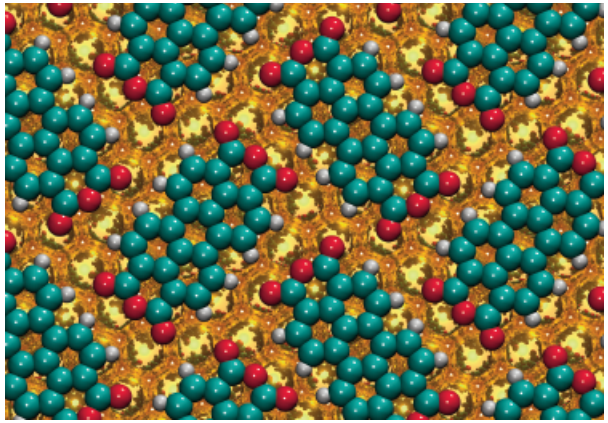
EMPA AKADEMIE

Zentrum für Wissenstransfer

Topical Day

Computational Modeling

Perspectives in Environmental and Materials Science



Empa, Dübendorf
Überlandstrasse 129

Thursday, June 17, 2010
09.30 to 17.00

Online registration
www.empa.ch/comp

Topic

Numerical simulation is nowadays considered the third main methodical approach in science, complementary to theory and experimental investigation. Born as a result of the development of approximate methods to numerically solve mathematical problems formulated in the theory, it today extends beyond its numerical analysis to direct modeling of systems and processes. This gives rise to the term "Computational Modeling".

Its development has always proceeded simultaneously to the evolution of Information and Communication Technologies and theoretical computer sciences.

However, a quantum leap in its widespread diffusion in natural sciences happened during the 1990s with the realization of parallel computers exploiting commodity off-the-shelf technology (COST). These computers, which start to be available in several scientific institutions, are known as "high-performance computer clusters". They consist of powerful computing "nodes" with a user-friendly interface, connected through an ultra-fast network and to a centralized high-end storage system.

The resulting architecture allows either to simultaneously run different independent tasks, which exploit huge stored data sets, or advanced large scale calculations requiring parallel algorithms.

Aims

This topical day aims to provide a representative introduction to Computational Modeling and an overview of the current high-performance computing facility available at Empa/Eawag, the **Ipazia** compute cluster.

In addition, this topical day supplies a detailed introduction to the Ipazia computing cluster's architecture and how to use it in your own research activity, with direct examples from its current experienced users.

Target Audience

This Topical Day is targeted at Empa's scientific and technical staff, PhD students and postdoctoral researchers.

Program

09.30 **Introduction**
Gian-Luca Bona, CEO Empa

09.45 **Ipazia: birth and growth of an Empa-Eawag computational aggregation point**
Daniele Passerone, Empa

10.15 **Coffee break**

10.40 **First-principles structure and property determination of materials for energy applications**
Riccarda Caputo, Empa

11.20 **Bottom-up design of graphene-derived nanostructures**
Stephan Blankenburg, Empa

12.00 **Lunch**

13.00 **Grain by grain. Molecular Dynamics investigation of granular friction and stick-slip in granular layers**
Michele Griffa, Empa

13.40 **Simulation of propagation of railway and aircraft noise**
Empa, Acoustics laboratory

14.20 **Coffee break**

14.50 **Honeycomb sandwich residual stress deformation pattern**
Gerald Kress, ETHZ

15.30 **A GIS-based tool for modelling large-scale crop-water relations**
Christian Folberth, Eawag

16.10 **Assessing the sources of air pollution in Europe with a high-resolution air quality model**
Dominik Brunner, Empa

General Information

Location
Empa, **AKADEMIE**
Überlandstrasse 129
CH-8600 Dübendorf

Costs
Topical Days are free of charge.

Registration
Online: **www.empa.ch/comp**

Registration Deadline
Thursday, June 10, 2010

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