EPFL Valais, ChE 602 Seminar, 13.04.2017

Title: The Times They Are a-Changin': A New Age for Computational Materials Science

Abstract:
The last 30 years have seen the steady and exhilarating development of powerful quantum simulation techniques, often based on density-functional theory, to understand, predict, or even design the properties of complex molecules or materials. Since these simulations are performed without any experimental input or parameter they can streamline, accelerate, or replace actual physical experiments. This is a far-reaching paradigm shift, substituting the cost- and time-scaling of brick-and-mortar facilities, equipment, and personnel with those, very different, of computing engines.

Nevertheless, computational science remains anchored to a renaissance model of individual artisans gathered in a workshop, under the guidance of an established practitioner. Great benefits could follow from rethinking such model, while adopting concepts and tools from computer science for the automation, management, preservation, analytics, and dissemination of these computational efforts.

I will offer my perspective on the current state-of-the-art in the field, its power and limitations, the role and opportunities of high-throughput computing, and some examples that hint at the novel approaches that are emerging.

Bio:
Nicola Marzari holds a degree in physics from the University of Trieste (1992) and a PhD in physics from the University of Cambridge (1996). He was a postdoctoral fellow at Rutgers University and a research scientist at the Naval Research Laboratory and at Princeton University (1996-01).

In 2001 he was appointed assistant professor of computational materials science at the Massachusetts Institute of Technology, where he was promoted to associate professor in 2005 and to the Toyota Chair of Materials Engineering in 2009. In 2010 he joined the University of Oxford as its first Statutory (University) Professor of Materials Modelling and director of the Materials Modelling Laboratory. He moved to EPFL in 2011, as chair of Theory and Simulation of Materials; from 2014 he also directs the MARVEL National Centre on Computational Design and Discovery of Novel Materials, a 12-year project involving 40 groups.