Institut für Numerische Simulation
Rheinische Friedrich-Wilhelms-Universität Bonn

hausdorff center for mathematics

Einladung zu einem Vortrag im Seminar
Materialwissenschaften und Mathematik

Prof. Dr. Ralf Drautz

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Ruhr-Universität Bochum, Germany

spricht zum Thema

From electrons to materials

Zeit: **Donnerstag, den 3. Februar 2011, 16.00 Uhr**

Ort: **Wegelerstrasse 6, Seminarraum 5.002**

gez. **Prof. Dr. Michael Griebel**, **Prof. Dr. Stefan Müller**

Abstract: While the fundamental laws for the description of materials are well established, the knowledge of the consequences of these laws for the behaviour of materials on the macroscopic scale is much more scarce. In fact, several orders in length and time need to be bridged in order to relate the mechanical behaviour of a material on the component scale to its electronic structure on the atomic length scale. This explains why new materials are hardly developed based on insight from Quantum Mechanics, but using traditional trial-and-error approaches that are supported by a large amount of experience and experimental evidence that has been accumulated over time. In my talk I will summarize the hierarchical structure of materials and highlight some of the challenges involved in bridging between the hierarchies. I will focus in particular on bridging the electronic to atomistic modelling hierarchies, where a quantum mechanical description needs to be simplified into interactions between classical particles. The relevance for the development of new alloys and steels will be briefly discussed.

The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) was set up three years ago with the aim of supporting the development and improvement of materials with modelling and simulation. ICAMS is supported by a consortium that comprises companies from steel and chemical industry.