

# HRVATSKO DRUŠTVO ZA MEHANIKU CROATIAN SOCIETY OF MECHANICS

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# Poziv

Pozivamo Vas na predavanje

## THE GENERALIZED ATOMIC-SCALE FINITE ELEMENT METHOD

koje će održati

Dr. -Ing. Jens Wackerfuß

Technische Universität Darmstadt, Njemačka

u utorak 07. rujna 2010. u 12:00 sati

na Fakultetu strojarstva i brodogradnje, Zagreb, Ivana Lučića 5, dvorana F.

Više o predavanju može se naći na web stranici: <a href="http://www.csm.hr">http://www.csm.hr</a>.

PREDSJEDNIK DRUŠTVA

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#### Title:

## THE GENERALIZED ATOMIC-SCALE FINITE ELEMENT METHOD

#### Abstact:

Atomic structures, exhibiting a physical dimension in the range of 1-100 nanometers, provide the basis for many novel applications in different fields of nanotechnology. However, before those structures can be applied, their mechanical behaviour has to be understood, so that reliable predictions can be made. In this context numerical methods, simulating the behaviour of atomic structures by using computers, play more and more a decisive role. The finite element method (FEM) is a reliable mathematical tool, in order to solve typical problems in solid mechanics. As it will be demonstrated in this talk, the FEmethod can - in principle - also be applied in the context of molecular mechanics. For this purpose the potential functions, describing the interaction between the atoms, have to be embedded into the formalism of the FEM. Thus, the structural analyses of atomic structures can be performed by using FE-codes. At the end of the talk some numerical examples will be presented; the main focus is placed on the investigation of the mechanical behaviour of carbon nanotubes.

# **Curriculum Vitae**

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University of California, Berkeley:

Post-doctoral fellow 01/2007-01/2008

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Group Leader MISMO since 09/2010 Senior Engineer 02/2008-08/2010

Post-doctoral fellow 2005-2006 Research and Teaching Assistant 2000-2005

Mann & Bernhardt, Engineering Consultants:

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Dr.-Ing. Civil Engineering (Ph.D. equivalent)

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