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Friedrich-Alexander-Universität
Erlangen-Nürnberg



Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

Freitag, **19.07.2013, 13:30 Uhr**, Egerlandstr. 5, Raum 0.044

On atomistic-continuum coupling for crystalline nano-structures:
from surface relaxations to localized inelastic mechanisms

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This talk presents the building blocks of a fully nonlocal quasicontinuum method based on adaptive finite element discretizations, cluster summation rules and energy-minimization algorithms. The method aims at a consistent, seamless nano-to-micro scale transition by atomistic-continuum (a-c) coupling at zero temperature. Beyond the description of the method's theoretical framework a focus of this talk is on the modeling of surface relaxation deformations and related stresses, which are the reason for size-dependent elasticity of e.g. nanowires. For this problem set we present solution strategies and their performance for a variation of cluster size, for h-uniform as well as h-adaptive mesh refinement. Nonstandard convergence results indicate the delicate interplay of physical effects with numerics.

As a second field of application we address some of the singular sets of solid mechanics at the nanoscale like localized inelastic deformation mechanisms that range from shear bands to cracks.

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