ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Institut de mathématiques des sciences computationnelles et ingénierie
MATHICSE

SEMINAIRE D'ANALYSE NUMERIQUE

- ***MERCREDI 23 Février 2011 à 16h15 à la salle MA A110***

Prof. ***CH. ORTNER*** *(UNIVERSITY OF OXFORD, U.K)* donnera une conférence intitulée:

"Consistency of atomistic/continuum coupling methods for crystalline solids"

Low energy equilibria of crystalline materials are typically characterised by localized defects that interact with their environment through long-range elastic fields. By coupling atomistic models of the defects with continuum models for the elastic far field one can, in principle, obtain models with near-atomistic accuracy at significantly reduced computational cost. However, several pitfalls need to be overcome to find a reliable coupling mechanism. Possibly the most widely discussed among these are the so-called "ghost forces" that typically arise in energy-based atomistic/continuum coupling mechanisms.
In this talk I will first describe the construction of energy-based atomistic/continuum coupling methods, how ghost forces arise, and how one can avoid them. I will then explain the resulting model errors due to different types of interface treatment. I will give partial answers to the fundamental question whether absence of ghost forces automatically implies "high accuracy" of the coupling scheme.

Lausanne, le 18 janvier 2011
Prof. Assyr Abdulle / nk

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Les séminaires qui ont lieu à la Section de Mathématiques sont annoncés sur Internet
(http://memento.epfl.ch/cgi-bin/memento/select?memento=MATHS)