Workshop "Multiscale simulations"

Host: Prof. Dr.-Ing. Stefan Diebels (Universität des Saarlandes)

Place: Universität des Saarlandes
Campus Saarbrücken, Building A2.3, Senatssaal, 1st Floor

Date: 9:30 - 16:30, 31/01/2014

The modelling of material involves multiple scales. In computational problems mechanical properties and structural behaviour are described in a range varying from atomistic scale, nanoscale or microscale to macroscale. On the fine scales, the size and orientation of local inhomogeneities influence the mechanical behaviour while on the coarse scale or macroscale the average behaviour has to be taken into account. Usually different methods are used to model the processes on the different scales, e.g. molecular dynamics can be applied to model the atomistic scale response while the finite element method can be used to describe the behaviour on the macroscale.

If specimens become smaller or the local inhomogeneities become stronger, processes on multiple scales start to interact. Therefore, it is one of the essential questions in the modelling how to bridge the gap between fine scale quantities, like atomistic or molecular deformations or local fine structures to macroscale quantities like stress and strain. Multiscale simulations, with such features as high efficiency of continuous models and considerable accuracy of microscale models, are promising methods to resolve this problem. Different scales are connected via upscaling processes, i.e. appropriate homogenization processes that are used to compute the average properties of the macroscopic model.

The following situations may occur in multiscale modelling:

- Single sided transference: Macroscopic properties of the material are computed on a small scale based on the locally inhomogeneous properties by homogenization techniques. The averaging is applied once and for all and the results are used on the macroscale.
- Multiple domains coupling: In a certain domain of interest a small scale model is used while in regions far away the macroscopic model is applied. The macroscopic properties should fit to the microscopic properties especially at the interface between the domains both models must fit together.
- Multilevel finite element modelling (FE^2): The constitutive relation of a macroscopic model is replaced by a microscopic model and an appropriate homogenization/projection method. In this case the coupling is two-sided because

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the macroscopic state influences the homogenization procedure while the homogenized microscopic model determines the macroscopic material behaviour.

- Seamless multiscale coupling techniques: Depending on the local properties the model can switch between a full resolution microscale model and a macroscale model. The seamless coupling is required not only on the multiple spatial scales but also on the temporal scales.

UniGR, intermatGR and Stefan Diebels are organizing a workshop entitled **"Multiscale simulations"**, bringing together **researchers, enterprises and experts** from the Greater Region.

We would like to invite you to the **one-day workshop** that will take place on 31/01/2014. **Workshop language** will be **English**.

AGENDA

9:30 - 9:45	Welcome (Uwe Hartmann, Vice-President for European and International Affairs, Universität des Saarlandes) Welcome, context and objectives of the meeting (Stefan Diebels, Universität des Saarlandes)
09:45 - 10:05	Microscale Simulation of real Al-Si alloys based on tomography data (Stefan Diebels/Michael Roland /Frank Mücklich/Anastasia Kruglova/Michael Engstler, Universität des Saarlandes) *(15 min. presentation, 5 min. discussion)*
10:05 - 10:25	A numerical FFT-based approach for continuum dislocation-based mechanics (Stéphane Berbenni/Vincent Taupin/Komlan Djaka/Claude Fressengeas, Université de Lorraine)
10:25 - 10:45	A multiscale theory of dislocation and disclination fields for polycrystal plasticity (Vincent Taupin/Claude Fressengeas, Université de Lorraine; Laurent Capolungo/Manas Upadhyay, G.W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology/CNRS, Metz)
10:45 - 11:05	Studies of structures and defects at atomic scale: metallic materials application (Jean-Marc Raulot, Université de Lorraine)
	- Coffee break –
11:20 - 11:40	Adaptive multiscale simulation of material failure: applications to molecular-dynamics/continuum coupling, polycrystalline materials and Hydrogen cutting of Silicon wafers (Stéphane Bordas, Université du Luxembourg/Pierre Kerfriden, Cardiff University)

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11:40 - 12:00 Multiscale Damage Simulation of Composites by Using the Lippmann-Schwinger Integral Equations (Heiko Andrä, Fraunhofer Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern)

12:00 - 12:20 Homogenization with propagation of instabilities through the different scales (Ludovic Noels, Université de Liège)

12:20 - 12:40 Multiscale models of membrane wrinkling (Michel Potier-Ferry, Université de Lorraine)

- Lunch -

13:30 - 13:50 Computing free energies of disordered systems (Tanja Schilling, Université du Luxembourg)

13:50 - 14:10 Multiscale Modelling of Adsorption in packed beds: effect of container geometry, packed bed configuration, grain shape and macropore structure of the adsorbent on the adsorption process (Kilian Schmidt, TU Kaiserslautern)

14:10 - 14:30 Extended Discrete Element Method for Multi-physics Applications (Bernhard Peters, Université du Luxembourg)

14:30 - 15:00 Presentation of funding possibilities: focus on Horizon 2020 (Corinna Hahn, Eurice, Saarbrücken)

- Coffee break -

15:15 - 16:30 Discussion on possible common projects

Conclusion and next steps

If you wish to participate (free of charge), contact Florian Weber fdweber@verw.uni-kl.de.

Please do not hesitate to contact us by e-mail, if you have any further questions: s.diebels@mx.uni-saarland.de and/orfdweber@verw.uni-kl.de.

The workshop belongs to a series of workshops organized by the "University of the Greater Region (UniGR)". Additional information about UniGR is available on www.uni-gr.eu or by contacting your local UniGR Officer(s) at Saarland University (c.hodyas@ugr.uni-saarland.de or n.ickert@ugr.uni-saarland.de), University of Liège (c.lebaron@ulg.ac.be), University of Luxembourg (kristina.hondrila@uni.lu), University of Lorraine (charlotte.tavernier@univ-lorraine.fr), University of Kaiserslautern (fdweber@verw.uni-kl.de) or Trier University (vieten@uni-trier.de).

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