Center for Computational Sciences and Simulation CCSS

UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

EXASTEEL – Bridging Scales for Multiphase Steels

SPP 1648
"Software for Exascale Computing"

The Priority Programme SPPEXA addresses fundamental research on the various aspects of High-Performance-Computing software. Its overall scientific objectives are the paradigm shift from sequential to massively parallel processing and the learning how to effectively and efficiently deal with commodity systems available in the future.

http://www.sppexa.de

Motivation

The project EXASTEEL in the SPP 1648 deals with the computational simulation of advanced high strength steels, incorporating phase transformation phenomena at the microscale using the FE^2 direct multiscale approach. Thereby in each macroscopic integration point an additional (microscopic) boundary value problem is solved and suitable volume averages of the microscopic responses replace the macroscopic constitutive set of equations compared to classical FEM computations, see e.g. [3]. In a serial set-up this procedure results in high numerical costs especially in the three dimensional case. New, highly efficient, parallel solver algorithms will enable the FE^2 approach to perform simulations of three dimensional multiscale material science problems. Due to the main objectives of SPPEXA, here the development for the exascale computing on future supercomputers is one of the main aspects.

Phase transformation and thermomechanics for FE^2

At the microscale representative volume elements (RVEs), see [2], are considered and the material behavior of the individual constituents is described by a finite plasticity model. In order to incorporate initial hardening distributions phase transformations of the original austenitic inclusions to martensite need to be modeled accurately and thus, a crystallographically motivated model is planned to be developed in the line of [4]. Phase transformations require the incorporation of thermo-mechanics into the FE^2 scheme and the derivation of associated consistent tangent moduli.

Parallel FE^2-framework

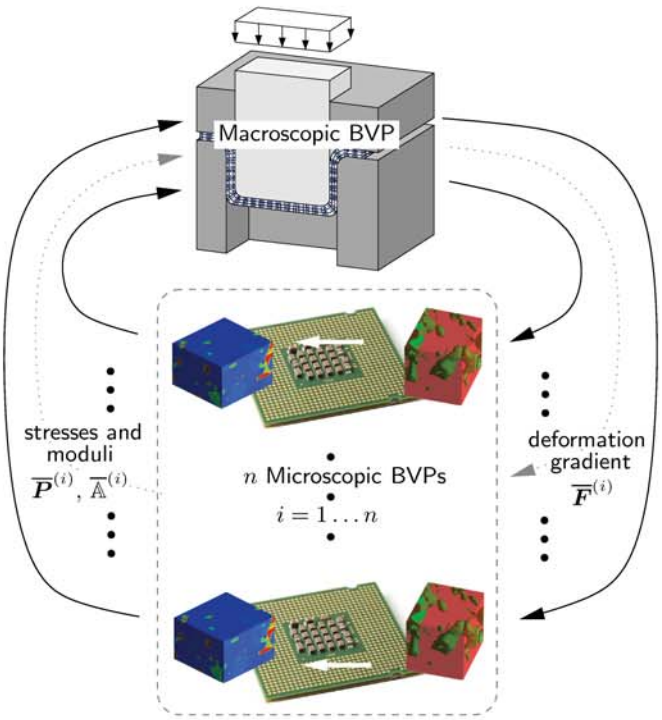
Parallelization on several levels is the central challenge in the focus of this research project. The level with the highest granularity is the parallel solution of the many RVE problems on the microscale. In the FE^2 method, at each macroscopic integration points the material response, i.e. the increment of the macroscopic first Piola-Kirchhoff stresses $\Delta\overline{\boldsymbol{P}}$, is calculated by

$$\Delta\overline{\boldsymbol{P}} = \overline{\mathbb{A}} : \Delta\overline{\boldsymbol{F}}\,,$$

with the macroscopic moduli $\overline{\mathbb{A}}$ and the increment of the macroscopic deformation gradient $\Delta\overline{\boldsymbol{F}}$. For the computation of the moduli $\overline{\mathbb{A}}$ using

$$\overline{\mathbb{A}} = \frac{1}{V}\int_{\mathcal{RVE}} \frac{\partial}{\partial\overline{\boldsymbol{F}}}\boldsymbol{P}(\overline{\boldsymbol{F}}+\widetilde{\boldsymbol{F}})\,dV$$

the solution of the microscopic boundary value problems are necessary, which in turns provide the microscopic field of the fluctuating part of the deformation tensor $\widetilde{\boldsymbol{F}}$. This results in a large number of trivially parallel simulations, see the illustration stated below. Algorithmically, this step has to be performed within the FEAP environment in such a way that an efficient further parallelization on the next level, i.e., on the level of each RVE, will be feasible.



Application software co-design

In co-designing the new application software for the simulation of high strength steels should be developed based on the domain decomposition algorithms and the FE^2 approach developed in the group of A. Klawonn and the group of J. Schröder, respectively. The software development will be performed using FEAP (Finite Element Analysis Program, R. Taylor, UC Berkeley). This package is originally not written for the use on large parallel computers, consequently, a wrapper environment has to be implemented.

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References

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