FE2TI: Computational Scale Bridging for Dual-Phase Steels

Motivation
Advanced High Strength Steels (AHSS) provide a good combination of both strength and formability and are therefore applied extensively in the automotive industry, especially in the crash relevant parts of the vehicle. Dual-phase (DP) steel is an example for such AHSS which is widely employed. The excellent macroscopic behavior of this steel is a result of the inherent micro-heterogeneity and complex interactions between the ferritic and martensitic phases in the microstructure. Thus, considering the microscale is indispensable for realistic simulations.

Radical Scale Bridging by FE²-Framework (FE2TI)
The FE²-method as illustrated for the Nakajima test below on the right, cf. [1, 2], is a direct multiscale method and provides a suitable numerical tool for radical scale bridging. We present our successful FE²-implementation FE2TI developed in the EXASTEEL project (SPPEXA), which we have scaled to 458 752 cores and $1.8 \times 10^6$ MPI ranks of JUQUEEN [3] and to the complete Mira (786K cores) at Argonne National Laboratory [4]. Inexact or exact FETI-DP methods are used to solve the 3D microscopic boundary value problems.

FE2TI Production Run on the Complete JUQUEEN
Results from a parallel FE2TI production run [4] considering a Neo-Hooke material and realistic steel microstructures. Each of the 1792 RVEs is decomposed into 512 FETI-DP subdomains. The simulation of 40 macroscopic load steps took approximately 5 hours.

Nonlinear Domain Decomposition Method
Nonlinear FETI-DP methods, developed in EXASTEEL, apply a decomposition-first paradigm (vs. classic linearization-first) and are based on the nonlinear saddle point problem [5],

$$\begin{align*}
\begin{bmatrix}
\tilde{K} & B^T \\
B & 0 
\end{bmatrix}
\begin{bmatrix}
\tilde{u} \\
\lambda 
\end{bmatrix}
&= 
\begin{bmatrix}
\tilde{f} \\
0 
\end{bmatrix} \\
B\tilde{u} &= 0.
\end{align*}
$$

The tangent $\tilde{K}$ is almost block diagonal. Nonlinear FETI-DP methods profit from increased local work, reduced communication & synchronization. Recently developed inexact nonlinear methods allow for inexact coarse solve by BoomerAMG using the global matrix (GM) or the local neighborhood (LN) approach [6, 7], where rigid body motions are interpolated exactly.

Strong Scaling of irNL-FETI-DP on Vulcan BG/Q
Strong scaling for a heterogeneous Neo-Hooke problem using inexact reduced nonlinear FETI-DP.

Weak Scaling of inNL-FETI-DP on JUQUEEN BG/Q
Weak scaling for a linear elastic beam problem (rectangular domain $[0, 8] \times [0, 1]$; clamped on the left; volume force applied in vertical direction) using inexact nonlinear FETI-DP and GM approach. This approach is purely iterative (without sparse direct solvers) and thus highly memory efficient.

Nakajima Test
An illustration of the FE² scale bridging method for the Nakajima test; averaging of Kirchhoff stresses $P$ on the microscale.