Bridging Scales for Multiphase Steels (EXASTEEL)

Motivation
The macroscopic behavior of advanced high strength steel is governed by the complex interactions of the individual constituents on the microscale. Simulations of challenging multiphase steel structural problems as the deep-drawing of automotive parts require accurate predictive material models incorporating the material’s microstructure evolution during the thermomechanical process.

Radical Scale Bridging by FE2-Framework
The FE2-method, cf. e.g. [1], is a direct multiscale method and provides a suitable numerical tool for radical scale bridging:

\[
\mathbf{\mathcal{F}} = \frac{1}{V} \int \mathbf{P} \, dV, \quad \mathbf{\mathcal{N}} = \frac{\partial \mathbf{\mathcal{F}}}{\partial \mathbf{F}} \left( \frac{1}{V} \int \mathbf{P} \, dV \right)
\]

However the computational requirements are still enormous in 3D and necessitate efficient algorithms at the exascale.

Mechanical Modeling at the Microscale
At the microscale 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 [3]. To derive a handable microscopic model an approach for the homogenization of different lattice orientations has to be developed, i.e.

\[
\sigma = \frac{1}{\omega} \int_{\Omega} \alpha(\vartheta_1, \vartheta_2, \vartheta_3) \vartheta \delta \tau_1 d\vartheta_1 d\vartheta_2 d\vartheta_3
\]

describes the stress state in the inclusion. Phase transformations require the incorporation of thermo-mechanics into the FE2-scheme and the derivation of associated consistent tangent moduli.

Parallel Application Software
Parallelization on several levels will be used to accomplish the scale bridging. The level with the highest granularity is the parallel solution of the many highly nonlinear RVE problems. The remaining orders of magnitude will be bridged by ultra-scalable solvers. The legacy application software FEAP will be used for the FE technology. A strong collaboration of all PIs is essential to create the correct infrastructure for all following steps. New ultra-scalable solvers for nonlinear problems will profit from an earlier DFG project on parallel nonlinear structural mechanics. The solvers will be based on FETI (Finite Element Tearing and Interconnecting) approaches thus reducing communication compared to other DD methods.

Solvers – Evolutionary Branch: Combine Domain Decomposition (DD) and Multigrid (MG) Methods
- (ir)FETI-DP-type DD methods have scaled to \(10^4 \rightarrow 10^5\) cores [4].
- Algebraic MG methods have scaled to \(10^3 \rightarrow 10^5\) cores [5].

<table>
<thead>
<tr>
<th>Method</th>
<th>Cores</th>
<th>dof</th>
<th>It</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>FETI-DP/boomerAMG</td>
<td>4,096</td>
<td>169M</td>
<td>18</td>
<td>30.1s</td>
</tr>
<tr>
<td></td>
<td>16,384</td>
<td>680.0M</td>
<td>16</td>
<td>30.6s</td>
</tr>
<tr>
<td></td>
<td>65,536</td>
<td>2,718.1M</td>
<td>16</td>
<td>35.7s</td>
</tr>
</tbody>
</table>

Recent FETI-DP algorithms [4] are methods to solve the linear saddle point problem:

\[
\begin{bmatrix}
\tilde{K} & B^T \\
B & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{u} \\
\lambda
\end{bmatrix} =
\begin{bmatrix}
\tilde{f} \\
0
\end{bmatrix},
\]

with a preconditioner

\[
\tilde{B}^{-1} =
\begin{bmatrix}
\tilde{K}^{-1} & 0 \\
M^{-1}B\tilde{K}^{-1} & -M^{-1}
\end{bmatrix}
\]

We will construct new, ultra-scalable Algebraic MG preconditioners as building blocks instead of direct solvers. The block \(\tilde{K}^{-1}\) will especially be tailored to profit from the decoupled structure of \(\tilde{K}\). Performance modeling and engineering will guide the development in a systematic process - years before exascale computers become available. Fault resilient AMG strategies will be applied.

Solvers – Revolutionary Branch: Nonlinear, nonoverlapping DD
Increased local work will reduce communication and the need for synchronization and thus also increase latency tolerance. Also facilitates the implementation of fault tolerance strategies. A successful overlapping nonlinear DD approach is known as ASPIN [6]. We, however, concentrate on nonoverlapping DD because of potentially smaller communication costs. We define nonlinear FETI-type methods as algorithms based on the nonlinear saddle point problem

\[
K(\mathbf{u}) + B^T\mathbf{\lambda} = f
\]

Here, \(K\) is decoupled such that the the tangent is block diagonal. The linearization of a nonlinear FETI-DD formulation can be written

\[
R_{\tilde{K}} \left(DK(R_{\tilde{u}}) \delta \tilde{u} + B_H^T \delta \tau \right) = R_{\tilde{K}}^T K(R_{\tilde{u}}) + B_H^T \mathbf{\lambda} - f
\]

\[
B^T \delta \tilde{u} = B \tilde{u},
\]

where the tangent \(DK\) is almost block diagonal. Different solution approaches are possible. Performance modeling and engineering are crucial for the best algorithmic choices. Building blocks will profit substantially from the evolutionary branch.

Performance Engineering: Profiling and Optimization
Performance measurements will be performed using LIKWID [7]. Early insights into performance limiting factors will enable algorithmic and software redesign. A white box approach will be taken for the performance optimization on the node level. The MPI+X approach will profit from expertise in hybrid parallelization models. Strategies increasing fault tolerance will be studied.