Materials Chain 2016

Dual Phase Steels – From Micro to Macro Properties (EXASTEEL-2)

Motivation

The macroscopic behavior of dual phase steels is governed by its structure on the microscale. To obtain a realistic model and to be able to predict material failure initiated at the microscopic level, crystal plasticity formulations have to be incorporated at the microscale, phenomenologically resolving an additional scale. The relevant phenomena, responsible for the properties of these steel materials, occur at a scale 10^4 to 10^6 times smaller than the macroscale.

Radical Scale Bridging by FE^2-Framework (FE2TI)

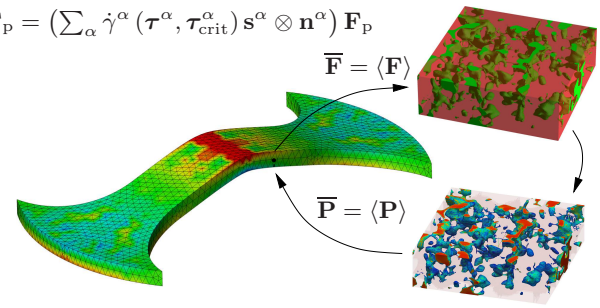
The FE^2-method as illustrated for the Nakajima test below, cf. [1, 2], is a direct multiscale method and provides a suitable numerical tool for radical scale bridging. We implemented a successfull FE^2 infrastructure in the project EXASTEEL, which we have scaled to 786 432 cores and 1.5m MPI ranks of Mira BG/Q at Argonne National Laboratory [3]. An inexact reduced FETI-DP method was used to solve the 3D microscopic boundary value problems.

FE2TI in 3D (Weak scaling)					
Cores	MPI ranks	#RVEs	Total dof	Time to Solution	Eff.
8 192	16 384	16	200M	914.34s	100.0%
16 384	32 768	32	401M	932.96s	98.0%
65 536	131 072	128	1.6B	929.35s	98.4%
131 072	262 144	256	3.2B	935.26s	97.8%
262 144	524 288	512	6.4B	937.78s	97.5%
524 288	1 048 576	1 024	12.8B	948.91s	96.4%
786 432	1 572 864	1 536	19.3B	943.81s	96.9%

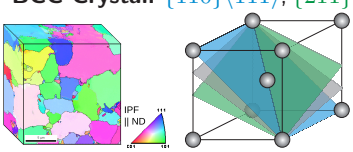
Crystal Plasticity - Nakajima Test

Crystal plasticity provides a finite strain plasticity framework which is crystallographically motivated and describes a physical polycrystalline texture evolution. Size effects in polycrystals can be described by concentrated hardening at grain boundaries.

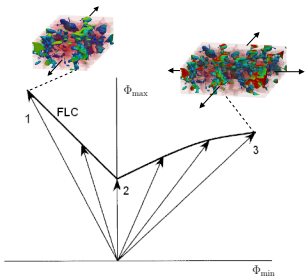
$$\dot{\mathbf{F}}_\mathrm{p} = \left(\sum_\alpha \dot{\gamma}^\alpha \left(\boldsymbol{\tau}^\alpha, \boldsymbol{\tau}^\alpha_\mathrm{crit}\right) \mathbf{s}^\alpha \otimes \mathbf{n}^\alpha\right) \mathbf{F}_\mathrm{p}$$



BCC Crystal: $\{110\}\langle\overline{1}11\rangle$, $\{211\}\langle\overline{1}11\rangle$, $\{321\}\langle\overline{1}11\rangle$



Virtual Lab - Predictive Simulations via Advanced Modeling



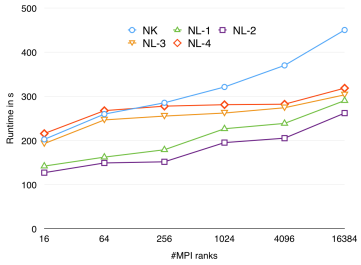
Forming limit curves characterize process limitation in sheet metal forming. Their determination is highly expensive due to the Nakajima experiments, each represents one point on the FLC. Thus, predictive simulations provide beneficial alternatives if efficient parallel algorithms are available.

Nonlinear Domain Decomposition Methods

Nonlinear FETI-DP methods (NL-1, NL-2), developed in EXASTEEL-1, apply a decomposition-first paradigm (vs. classic linearization-first (NK)) and are based on the nonlinear saddle point problem [4],

$$\begin{aligned} \widetilde{K}(\tilde{u}) + B^T\lambda &= \tilde{f} \\ B\tilde{u} &= 0\,. \end{aligned} \tag{1}$$

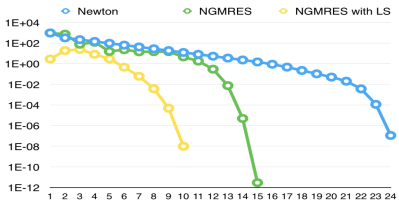
The tangent $D\widetilde{K}$ is almost block diagonal. Parallel scalability to 786 432 cores on Mira was shown for an inexact NL-1 approach.



New NL-3 and NL-4 methods [5] perform a partial nonlinear elimination of u_B or u_I before linearizing (1). Methods profit from **increased local work**, **reduced communication & synchronization** and allow for **inexact coarse solve** by BoomerAMG [6].

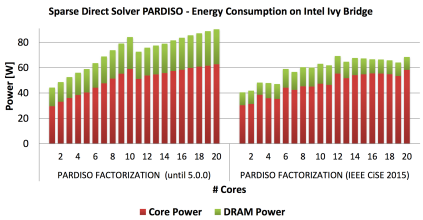
Composing Nonlinear Solvers

Combining our nonlinear FETI-DP methods with different nonlinear solvers, as NGMRES or Anderson Acceleration, can reduce the number of global iterations and thus the time to solution.



In [7], different nonlinear solvers have already been composed successfully. We will leverage the PETSc framework for the composition of nonlinear solvers [7]. Using different globalization approaches can additionally enhance the robustness of the methods, allowing the use of larger load steps, while still keeping the good scalability properties.

Performance Engineering (PE) for BoomerAMG and PARDISO



The important building blocks BoomerAMG and PARDISO will be considered as white boxes allowing PE and use of a-priori information. Performance will be measured using LIKWID [8] to improve the node-level performance. A detailed performance model will be established for the two most-important PARDISO steps: **sparse LU factorization** and **forward-backward substitution**. Information available from the domain-decomposition preconditioner will be used to improve pivoting in PARDISO and construction of coarse operators in BoomerAMG resulting in a **strong coupling of PARDISO, BoomerAMG and FETI-DP**. New algorithms for a **fast** and **energy efficient** computation of a Schur complement will be used, cf. [9]; further performance advances of PARDISO by SIMD and accelerators.

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