Priority Programme 1648
Software for Exascale Computing
DFG Deutsche Forschungsgemeinschaft

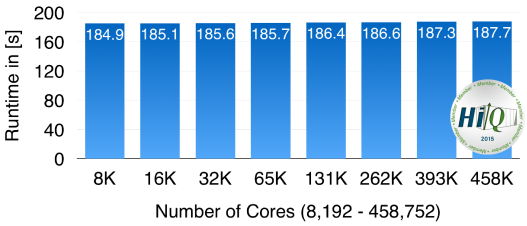
Dual Phase Steels – From Micro to Macro Properties (EXASTEEL-2)

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 (FE^{2}TI)

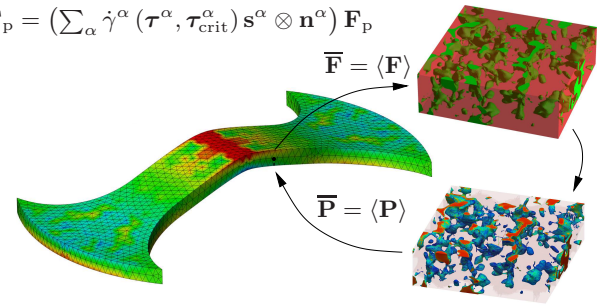
The FE^2-method as illustrated for the Nakajima test below, cf. [1, 2], is a direct multiscale method and provides a suitable numerical tool for radical scale bridging. We will build on our successfull FE^2 infrastructure from EXASTEEL-1, which we have scaled to 458 752 cores and 1.8m MPI ranks of JUQUEEN [3]. An inexact reduced FETI-DP method was used to solve the 3D microscopic boundary value problems.



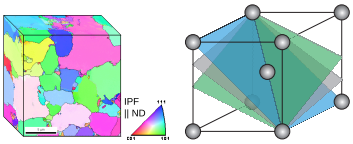
Crystal Plasticity - Nakajima Test

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.

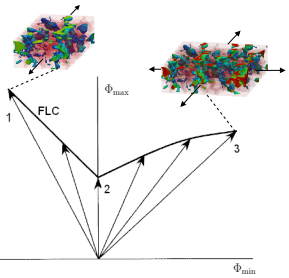
$$\dot{\mathbf{F}}_\mathrm{p} = \left(\sum_\alpha \dot{\gamma}^\alpha\left(\boldsymbol{\tau}^\alpha, \boldsymbol{\tau}^\alpha_\mathrm{crit}\right)\mathbf{s}^\alpha \otimes \mathbf{n}^\alpha\right)\mathbf{F}_\mathrm{p}$$



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



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.

A New Nonlinear Domain Decomposition Method

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

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

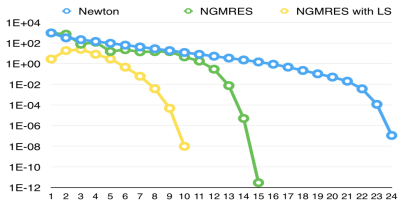
The tangent $D\widetilde{K}$ is almost block diagonal. Parallel scalability to 262 144 cores on Mira was shown.

New inexact reduced Nonlinear-FETI-DP-2-approach applies partial nonlinear elimination $u_B = h(\tilde{u}_\Pi, \lambda)$ before linearizing (1). Methods profit from **increased local work**, **reduced communication & synchronization**. New method allows for **inexact coarse solve** by BoomerAMG [5] and signicantly reduces number of **AMG setups**.

N	Solver	Krylov It.	Local Setup	Coarse Setup	N	Krylov It.	Local Setup	Coarse Setup
4	NK-FETI-DP (old)	34	14	14	16	122	15	15
	NL-FETI-DP-2 (EXASTEEL-1)	**6**	14	14		**27**	19	19
	NL-FETI-DP-1 (EXASTEEL-1)	5	15	15		45	19	19
	irNL-FETI-DP-2 (new)	**7**	19	**3**		**34**	25	**4**
64	NK-FETI-DP (old)	238	17	17	256	290	19	19
	NL-FETI-DP-2 (EXASTEEL-1)	**47**	23	23		**54**	23	23
	NL-FETI-DP-1 (EXASTEEL-1)	90	22	22		83	23	23
	irNL-FETI-DP-2 (new)	**72**	30	**5**		**62**	32	**4**

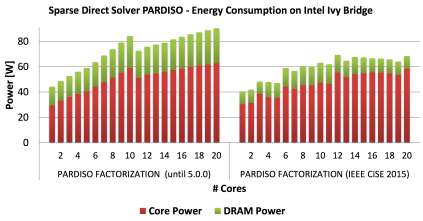
Composing Nonlinear Solvers

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 [6], different nonlinear solvers have already been composed successfully. We will leverage the PETSc framework for the composition of nonlinear solvers [6]. 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 [7] 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. [8]; further performance advances of PARDISO by SIMD and accelerators.

[1] Schröder, J.; Hackl K. [2014], Plasticity and Beyond, CISM.
[2] Balzani, D.; Gandhi, A.; Tanaka, M.; Schröder, J. [2015]
[3] Lanser, M.; Klawonn, A..; Rheinbach, O. [2015]
[4] Klawonn, A.; Lanser, M.; Rheinbach, O. [2014a,2014b]
[5] Baker, A.; Falgout, R.; Kolev, T.; Meier-Yang, U. [2012]
[6] Brune, P.; Knepley, M.G.; Smith; B.F.; Tu, X. [2013]
[7] Treibig, J.; Hager, G.; Wellein, G. [2010]
[8] Anitescu, M.; Petra, C. G.; Schenk, O. [2014]

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