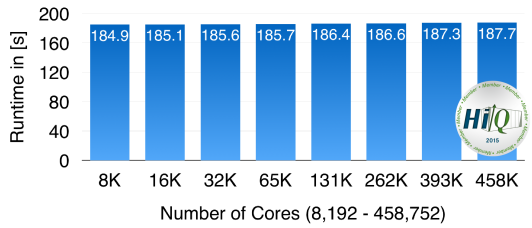
FE2TI: Computational Scale Bridging for Dual-Phase Steels

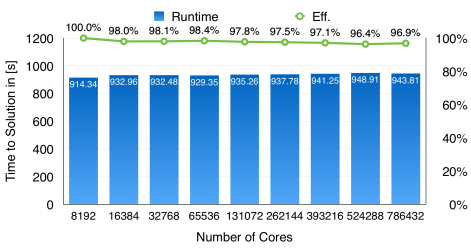
Motivation

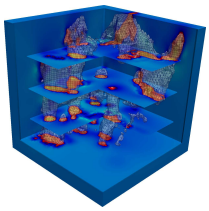
Advanced High Strength Steels (AHSS) provide a good combination of both strength and formability and are therefore applied extensively in the automotive industry, especially in the crash relevant parts of the vehicle. Dual-phase (DP) steel is an example for such AHSS which is widely employed. The excellent 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 FE^2-Framework (FE2TI)

The FE^2-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 successfull FE^2 implementation FE2TI developed in the EXASTEEL project (SPPEXA), which we have scaled to 458 752 cores and 1.8×10^6 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.

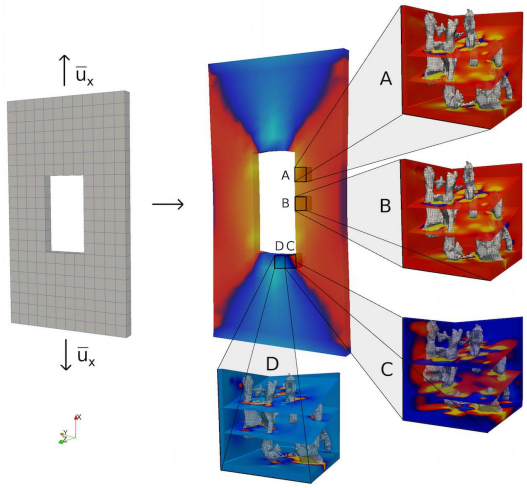




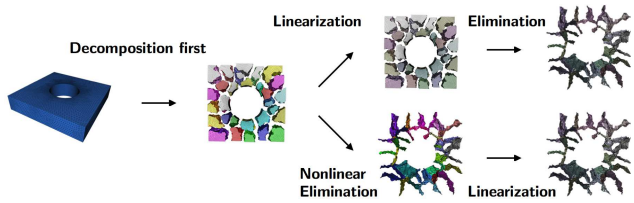


FE2TI Production Run on the Complete JUQUEEN

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],

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

The tangent $D\widetilde{K}$ 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.

Cores	Subdomains	Problem Size	Execution Time	Actual Speedup	Parallel Effic.
1 024	131 072	419 471 361	3 365.1s	1.0	100%
4 096	131 072	419 471 361	868.0s	3.9	97%
16 384	131 072	419 471 361	231.4s	14.6	91%
65 536	131 072	419 471 361	64.3s	51.6	81%
131 072	131 072	419 471 361	41.7s	80.6	63%

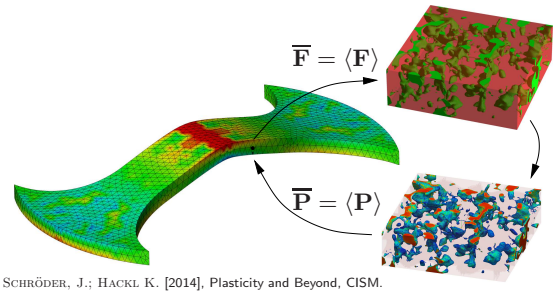
Weak Scaling of iNL-FETI-DP on JUQUEEN BG/Q

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.

# MPI ranks	Problem Size	Krylov It.	Execution Time	Time GMRES	Parallel Effic.
32	1 644 162	27	51.4s	32.6s	100%
512	26 237 442	23	49.5s	30.3s	104%
8 192	419 522 562	20	44.1s	24.5s	117%
131 072	6 711 255 042	20	46.5s	24.6s	111%
524 288	26 844 282 882	22	56.9s	27.8s	90%
917 504	46 977 433 602	24	65.2s	30.3s	79%

Nakajima Test

An illustration of the FE^2 scale bridging method for the Nakajima test; averaging of Kirchhoff stresses $\mathbf{P}$ on the microscale.



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