# EXASTEEL-II

# Multiscale contact simulations of steel using FE2TI


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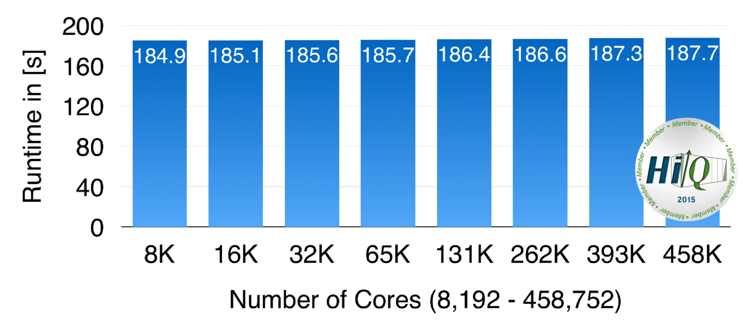
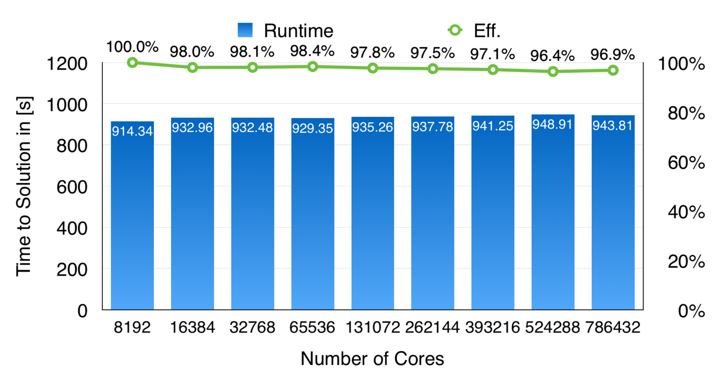
## Introduction

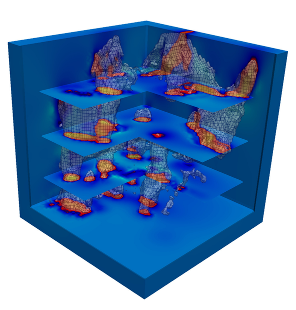
Advanced High Strength Steels (AHSS) provide a good combination of both strength and formability and are therefore applied extensively in the automotive industry, especially in the crash relevant parts of the vehicle. Dual-phase (DP) steel is an example for such AHSS which is widely employed. The excellent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

## Scale Bridging by FE$^2$-Framework (FE2TI)

The FE$^2$-method as illustrated for the Nakajima test in the box *Forming Limit Curves* on the right, cf. [1, 2], is a direct multiscale method and provides a suitable numerical tool for radical scale bridging. The macroscopic material model is replaced by averaged stresses and tangent moduli on the microscale. We present our successfull FE$^2$ implementation FE2TI developed in the EXASTEEL project (SPPEXA), which we have scaled to 458 752 cores and $1.8 \times 10^6$ MPI ranks of JUQUEEN [3] and to the complete Mira (786K cores) at Argonne National Laboratory [4] for hyperelasticity problems already in 2015. Inexact or exact FETI-DP methods are used to solve the 3D microscopic boundary value problems.



## Isoparametric Contact Element

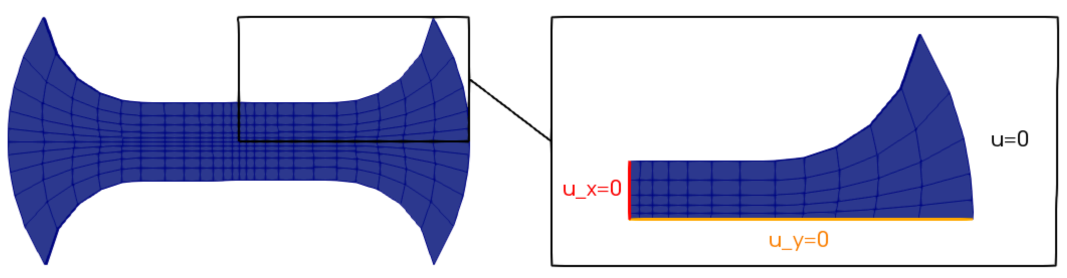
With quadratic shape functions, additional terms in the rhs and stiffness matrix for an active FE-node $i$:

$$\mathbf{rhs_i} = \int_{-1}^{1}\int_{-1}^{1} \varepsilon_N \cdot g_N(\xi,\eta) \cdot N_i(\xi,\eta) \cdot \vec{n} \; d\xi \; d\eta,$$

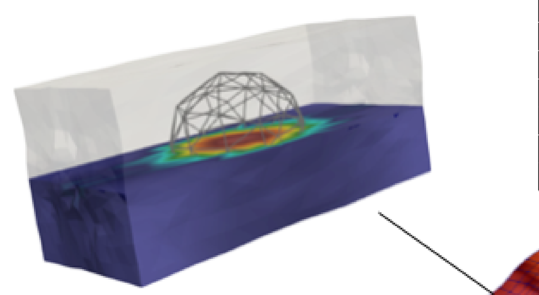
$$\mathbf{K_{ik}} = \int_{-1}^{1}\int_{-1}^{1} \varepsilon_N \; N_i(\xi,\eta) \; N_k(\xi,\eta) \cdot \vec{n}\vec{n}^T \; d\xi \; d\eta.$$

## Numerical Results

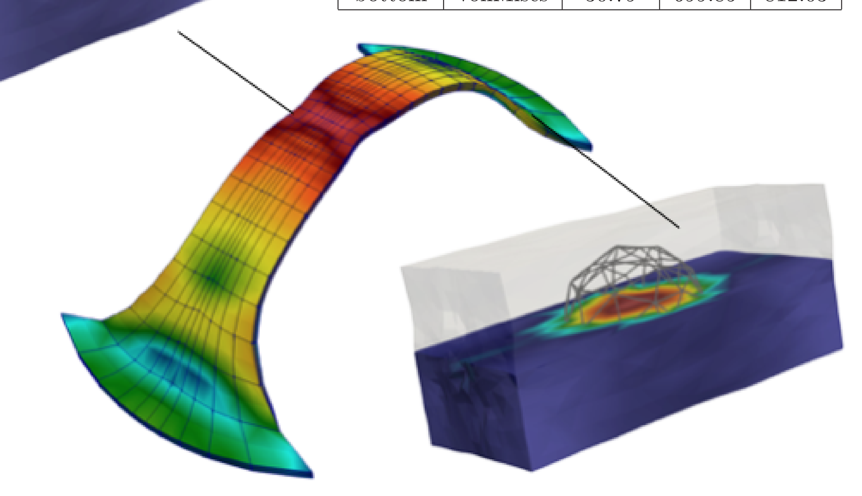
We have performed a simulation with a specimen of the Nakajima test on magnitUDE using the FE$^2$ method with direct solvers on the microscale.




- Comp. time ≈ 10h
- $\varepsilon_N = 500$
- MPI ranks: 4860 (use of symmetry)
- $r_{\text{Tool}} = 59$
- Macro: $118 \times 33.34 \times 2$ with $12 \times 5 \times 3$ Q2 FE
- Micro: 941 P2 FE, spherical inclusion $(r = 0.3)$

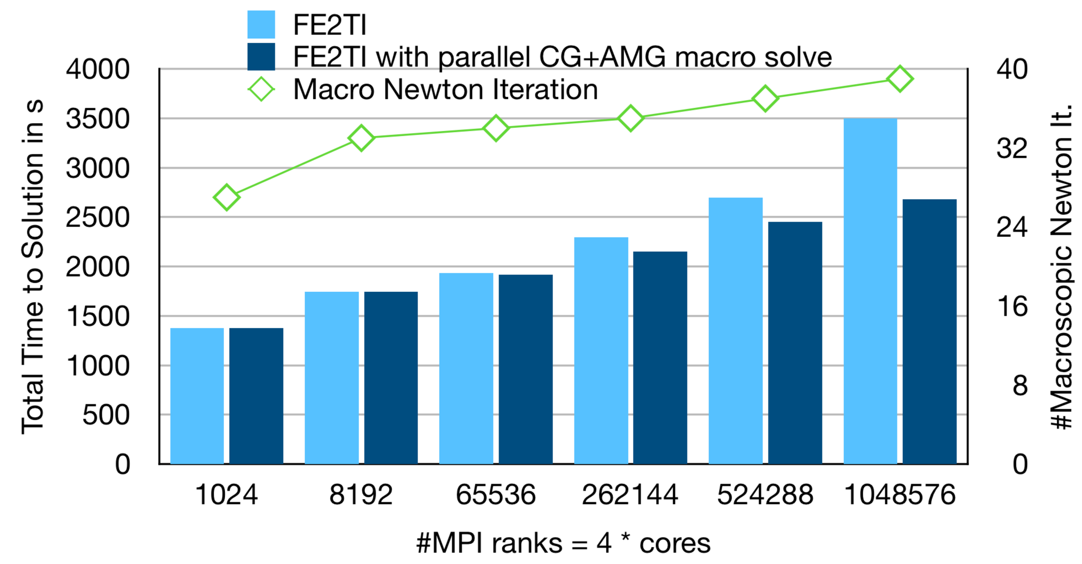


| | | Load step | | |
|---|---|---|---|---|
| | | 1 | 417 | 614 |
| | Sphere | 0.1 | 27.35 | 30.38 |
| **Center** top | Displ. $z$ | 8.52e-2 | 27.06 | 29.51 |
| | vonMises | 37.05 | 708.91 | 807.97 |
| **Center** bottom | Displ. $z$ | 8.52e-2 | 27.33 | 30.44 |
| | vonMises | 30.79 | 699.85 | 812.03 |



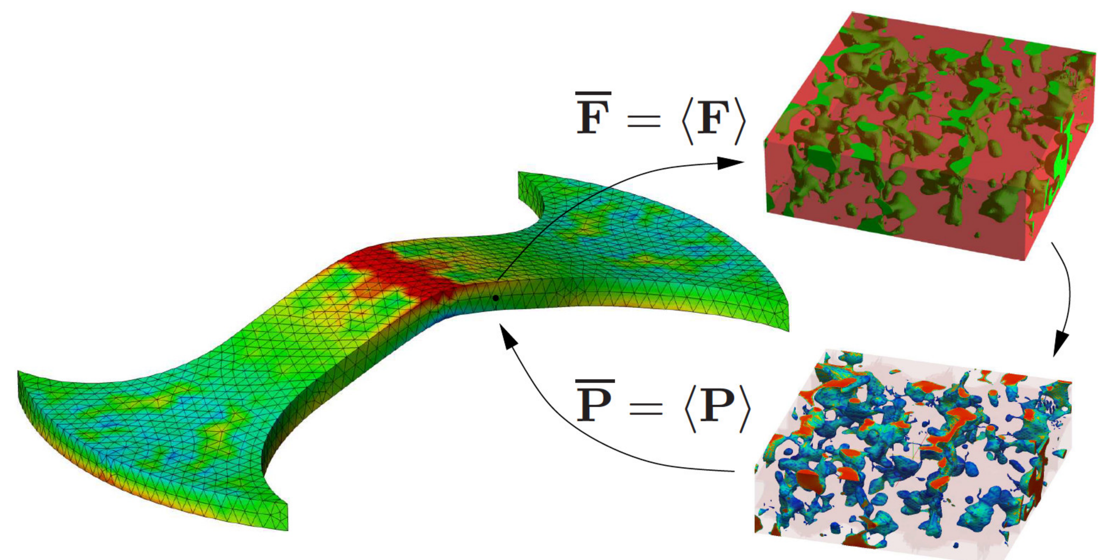
## Parallel Scalability for a Realistic Setup Using a Parallel Macro Solver

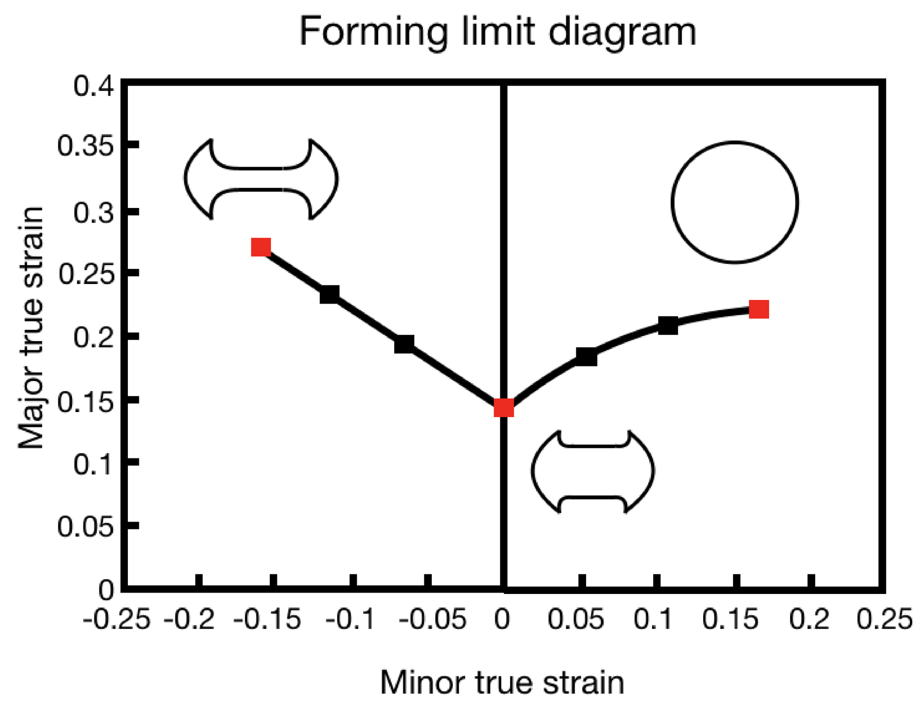
If the macroscopic problem is large, a parallelization is necessary. We recently included the option to use CG with a BoomerAMG preconditioner [5] on the macroscale instead of using sparse direct solvers. Using **917,504 MPI ranks on the complete JUQUEEN for a FE2TI production simulation** (unstructured RVEs, an J2-elasto-plasticity material model, several load steps, a large macroscopic deformation problem with 14K degrees of freedom), the time to solution can be reduced by a factor of 1.3. We also include a scaling graph for a similar realistic setup.




## Forming Limit Curves

The maximum formability of steels for different stress states is summarized in a forming limit curve (FLC). **The most common material test to determine FLCs is the Nakajima test**, where the rigid tool is the upper half of a sphere and the sheet metal is clamped between blank holder and die; see below for an illustration.




**To predict the FLC of a given microstructure, the contact formulation in the context of FE$^2$ is indispensable.**

## Frictionless Contact - The Penalty Method

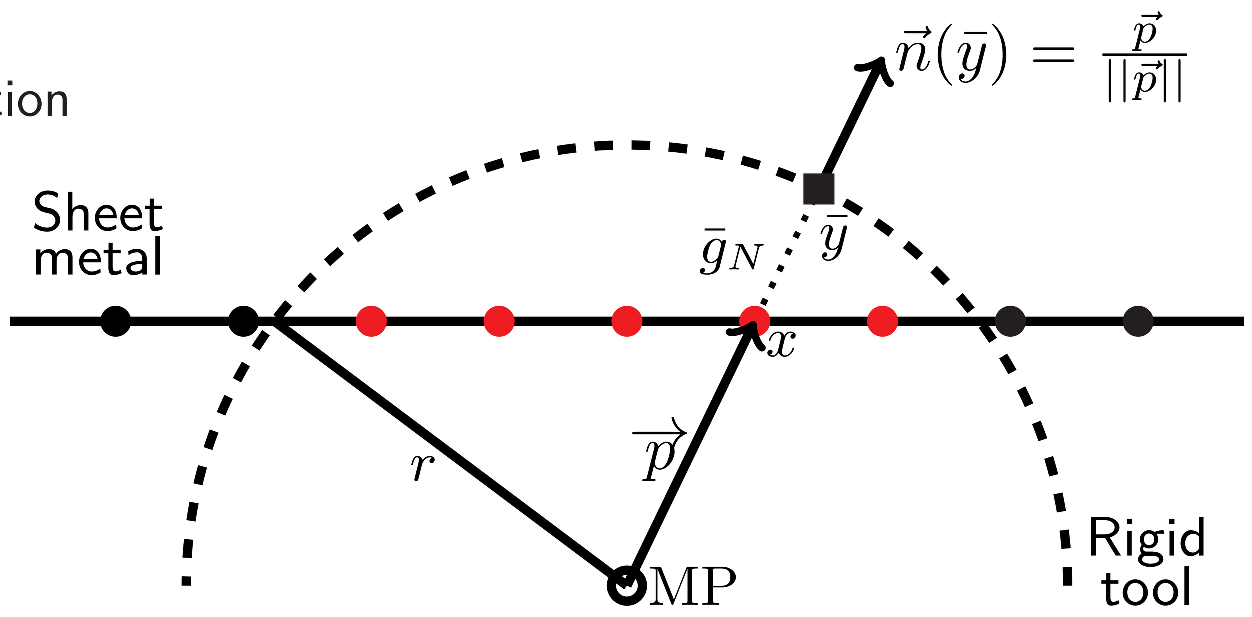
- Use of penalty method does not increase the number of unknowns
- Larger penalty parameter $\varepsilon_N > 0$ enforces contact constraints more precisely but increases condition number
- Only contact constraints in normal direction

■ $\bar{y}$ Point on the rigid tool surface with minimal distance to FE-node $x$

● FE-node with active contact constraint (red)

● FE-node with inactive contact constraint (black)

$$\bar{g}_N = \begin{cases} (x - \bar{y}) \cdot \vec{n}(\bar{y}) & \text{if } (x - \bar{y}) \cdot \vec{n}(\bar{y}) < 0 \\ 0 & \text{otherwise.} \end{cases}$$




**Active contact constraints add** $\frac{1}{2}\int_{\Gamma_c} \varepsilon_N (\bar{g}_N)^2 \, dA$ **to the energy functional**; see [6].

## References


[1] J. Schröder. A numerical two-scale homogenization scheme: the FE2-method. In J. Schröder and K. Hackl, editors, *Plasticity and Beyond: Microstructures, Crystal-Plasticity and Phase Transitions*, pages 1–64. Springer Vienna, Vienna, 2014.

[2] D. Balzani, A. Gandhi, M. Tanaka, and J. Schröder. Numerical calculation of thermo-mechanical problems at large strains based on complex step derivative approximation of tangent stiffness matrices. *Comp. Mech.*, 55:861–871, 05 2015.

[3] A. Klawonn, M. Lanser, and O. Rheinbach. Exasteel - computational scale bridging using a FE2TI approach with ex_nl/FE$^2$. In *JUQUEEN Extreme Scaling Workshop 2015*, 2015. Technical Report.

[4] A. Klawonn, M. Lanser, and O. Rheinbach. FE2TI: Computational scale bridging for dual-phase steels. In *Proceedings of ParCo 2015*, volume 27 of *IOS Series: Advances in Parallel Computing*, pages 797–806, 2016. Parallel Computing: On the Road to Exascale.

[5] A. H. Baker, A. Klawonn, T. Kolev, M. Lanser, O. Rheinbach, and U. Meier Yang. Scalability of classical algebraic multigrid for elasticity to half a million parallel tasks. In *Software for Exascale Computing - SPPEXA 2013-2015*, pages 113–140. Springer International Publishing, Cham, 2016.

[6] P. Wriggers. *Computational Contact Mechanics.* John Wiley & Sons, LTD, 2002.