Scalable Nonlinear Domain Decomposition Methods

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Based on joint work with
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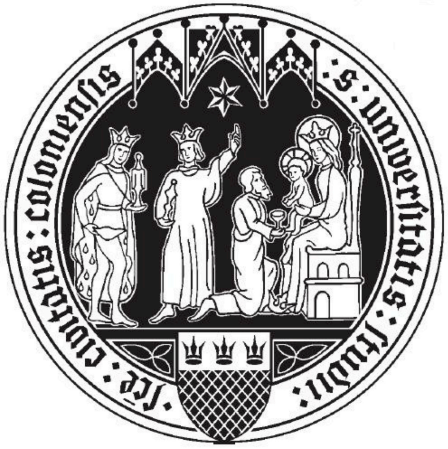
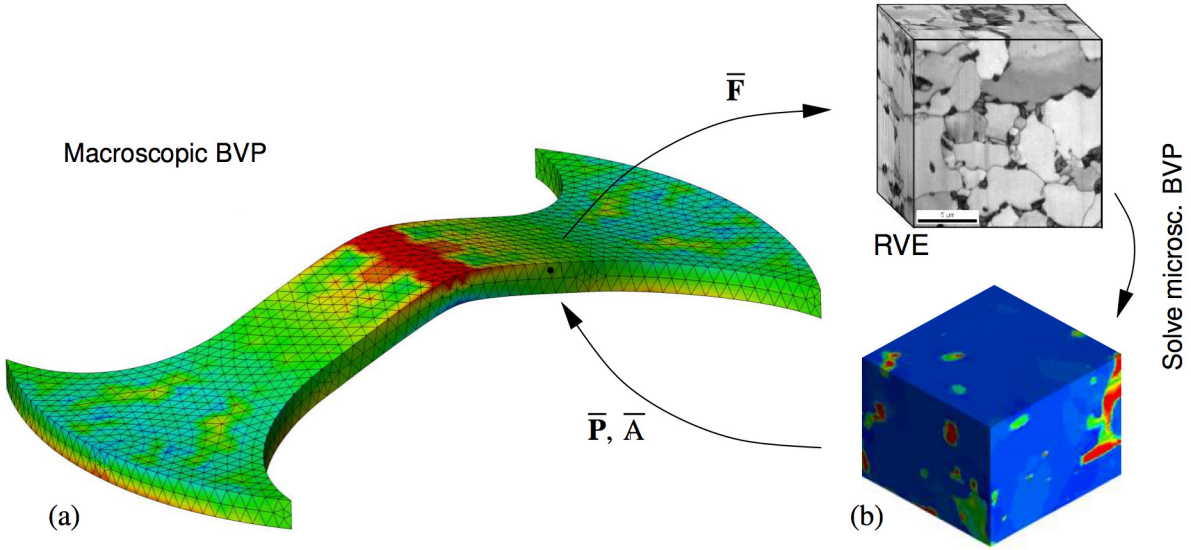


EXASTEEL - Bridging Scales for Multiphase Steels



Principal Investigators

- A. Klawonn, U Cologne
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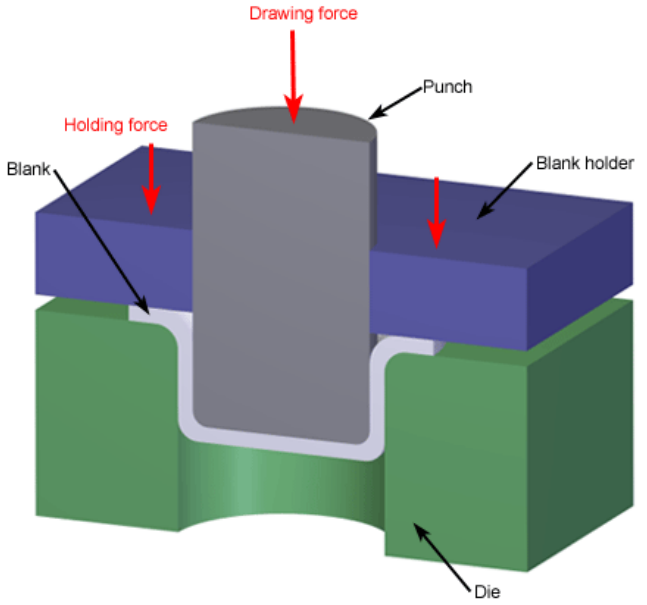
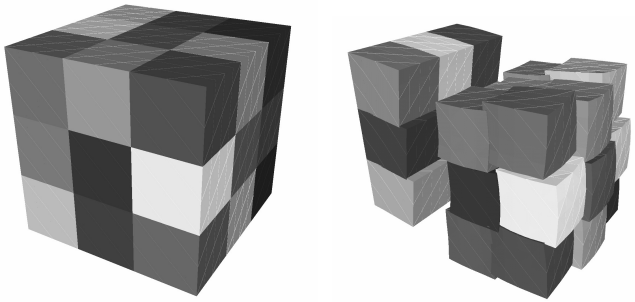
- Challenging 3D multiscale problems from nonlinear structural mechanics with plasticity.
- Highly concurrent computational scale bridging in continuum mechanics (FE2)
- Parallel FE2 implementation FE2TI based on PETSc and BoomerAMG
- Hybrid domain decomposition/multigrid implicit solvers for nonlinear problems



Efficient Parallel Solver: FETI-DP

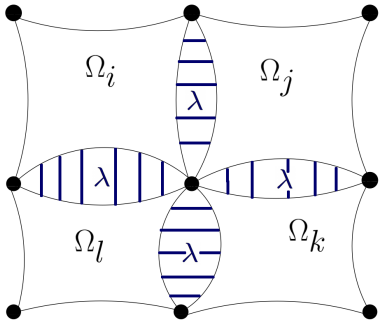
Finite Element Tearing and Interconnecting - Dual-Primal

Divide and Conquer Algorithm: Decompose computational domain into N nonoverlapping subdomains.
FETI-DP coarse space: Strong coupling in few degrees of freedom.



$$\begin{bmatrix} K_{BB}^{(1)} & & & \widetilde{K}_{\Pi B}^{(1)T} \\ & \ddots & & \vdots \\ & & K_{BB}^{(N)} & \widetilde{K}_{\Pi B}^{(N)T} \\ \widetilde{K}_{\Pi B}^{(1)} & \cdots & \widetilde{K}_{\Pi B}^{(N)} & \widetilde{K}_{\Pi\Pi} \end{bmatrix} =: \begin{bmatrix} K_{BB} & \widetilde{K}_{\Pi B}^T \\ \widetilde{K}_{\Pi B} & \widetilde{K}_{\Pi\Pi} \end{bmatrix}.$$

Introduce Lagrange multipliers and enforce zero jump between subdomains: $B_B u_B = 0$



$$\begin{bmatrix} K_{BB} & \widetilde{K}_{\Pi B}^T & B_B^T \\ \widetilde{K}_{\Pi B} & \widetilde{K}_{\Pi\Pi} & O \\ B_B & O & O \end{bmatrix} \begin{bmatrix} u_B \\ \tilde{u}_\Pi \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} f_B \\ \tilde{f}_\Pi \\ 0 \end{bmatrix}$$

In compact form:

$$\begin{bmatrix} \widetilde{K} & B^T \\ B & O \end{bmatrix} \begin{bmatrix} \tilde{u} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \tilde{f} \\ 0 \end{bmatrix}$$

Classical FETI-DP Algorithm

First reducing to the Lagrange multipliers:

$$\boxed{F\boldsymbol{\lambda} = d}$$

$$F = \underbrace{B_B K_{BB}^{-1} B_B^T}_{\text{local solvers}} + \underbrace{B_B K_{BB}^{-1} \widetilde{K}_{B\Pi} \widetilde{S}_{\Pi\Pi}^{-1} \widetilde{K}_{\Pi B} K_{BB}^{-1} B_B^T}_{\text{coarse problem; coupled!}}.$$

$\mathbf{B_B}$: Communication over the interface.
$\mathbf{K_{BB}^{-1}}$: Local direct solvers.
$\widetilde{\mathbf{S}}_{\mathbf{\Pi\Pi}}^{\mathbf{-1}} := \widetilde{\mathbf{K}}_{\mathbf{\Pi\Pi}} - \widetilde{\mathbf{K}}_{\mathbf{\Pi B}} \mathbf{K}_{\mathbf{BB}}^{\mathbf{-1}} \widetilde{\mathbf{K}}_{\mathbf{\Pi B}}^{\mathbf{T}}$: Exact solution of a global problem $\Rightarrow$ scaling bottleneck

The Preconditioner

Preconditioner: $M^{-1} := B_{D,\Delta} S B_{D,\Delta}^T$ (Sum of local operators)

1. S Schur complement of K (Interior variables eliminated). Local solvers.
2. $B_{D,\Delta}$ appropriately scaled jump operator (scaling depends on pde coeff.)

FETI-DP is PCG solving

$$M^{-1} F\boldsymbol{\lambda} = M^{-1} d$$

Newton-Krylov FETI-DP

Classical use of FETI-DP in the context of nonlinear finite element problems:

For a nonlinear problem arising from a discretization of a nonlinear partial differential equation

$$A(u) = 0$$

we linearize first with a Newton method

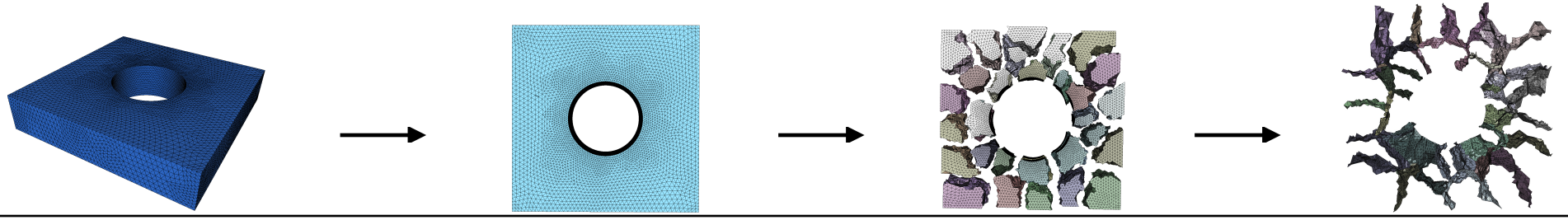
$$u^{(k+1)} = u^{(k)} - \alpha^{(k)} \delta u^{(k)}$$

with a step length $\alpha^{(k)}$, and the update $\delta u^{(k)}$ is given by:

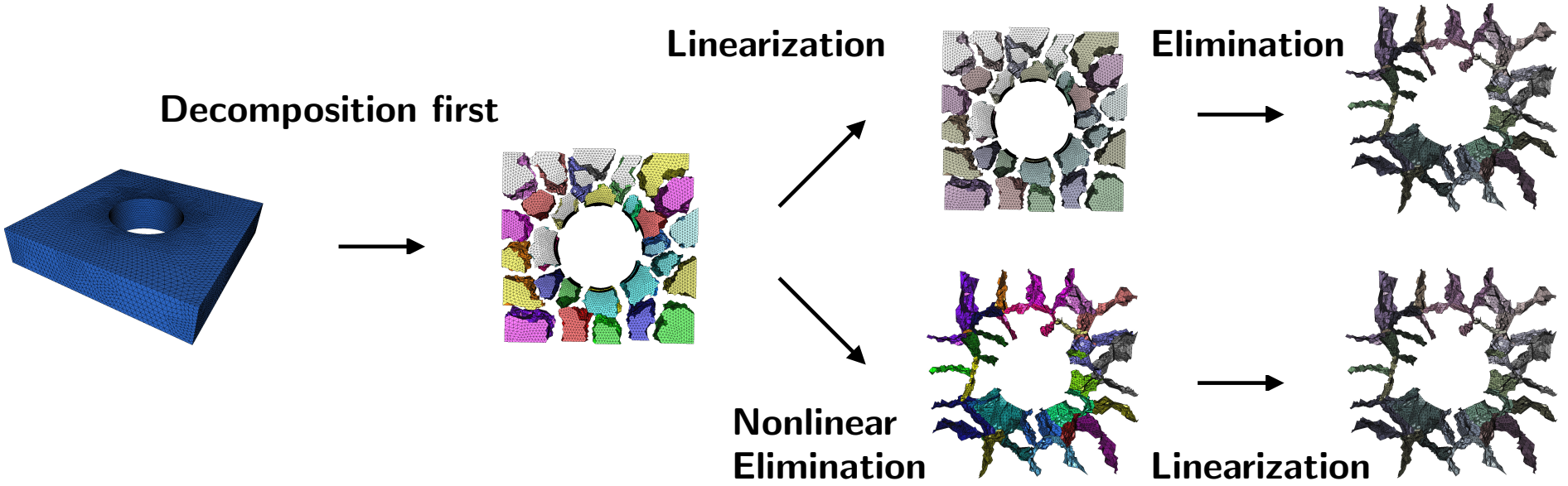
$$DA(u^{(k)})\delta u^{(k)} = A(u^{(k)}). \tag{1}$$

Newton-Krylov FETI-DP is decomposing the computational domain and using a FETI-DP type method in order to solve (1).

Linearize first **Decomposition** **Elimination**



Nonlinear FETI-DP Methods

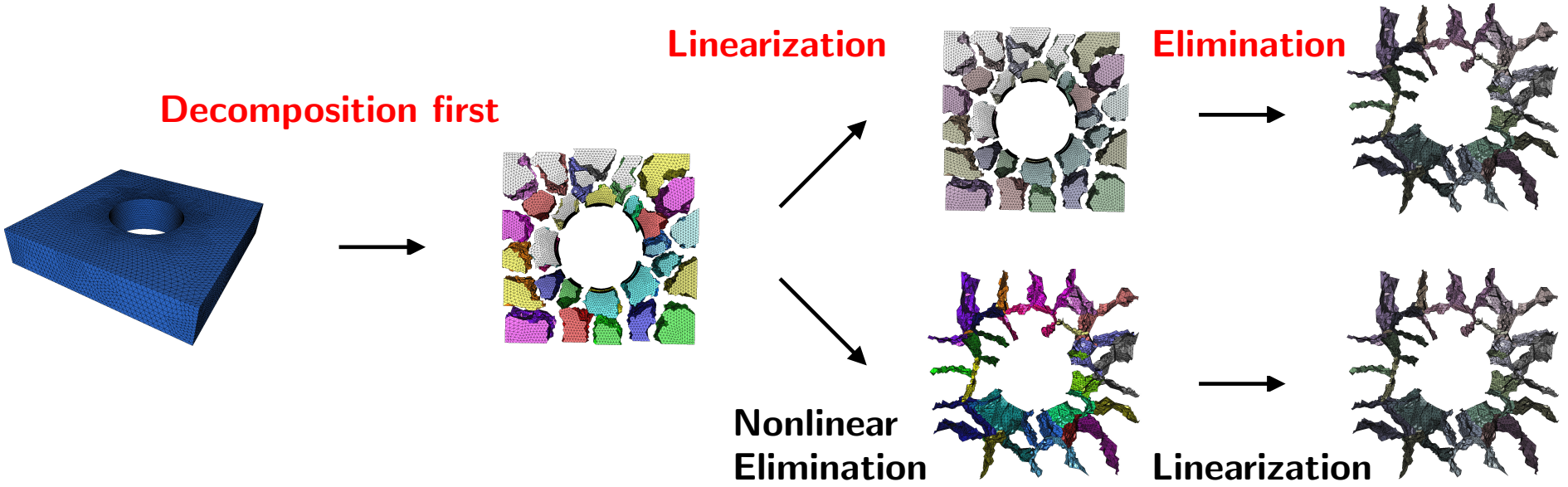


- Decomposition of the discretized nonlinear problem before linearization
- $\Rightarrow$ local nonlinear problems $\Rightarrow$ Increased local work
- Reduced number of Newton steps, Krylov iterations, and communication
- Combinable with hybrid FETI-DP/Multigrid methods

All nonlinear FETI-DP methods are based on the nonlinear FETI-DP saddlepoint system:

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

Nonlinear FETI-DP Methods - Linearize First



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Nonlinear FETI-DP Methods - Linearize First

Based on the nonlinear master system

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

the Newton linearization with respect to $(\tilde{u}, \lambda)$ results in the linear system

$$\begin{bmatrix} D\widetilde{K}(\tilde{u}) & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \delta\tilde{u} \\ \delta\lambda \end{bmatrix} = \begin{bmatrix} \widetilde{K}(\tilde{u}) + B^T\lambda - \tilde{f} \\ B\tilde{u} \end{bmatrix}. \tag{2}$$

With splitting up $\delta\tilde{u} = (\delta u_B^T, \delta\tilde{u}_\Pi^T)^T$:

$$\begin{bmatrix} DK_{BB} & D\widetilde{K}_{\Pi B}^T & B_B^T \\ D\widetilde{K}_{\Pi B} & D\widetilde{K}_{\Pi\Pi} & 0 \\ B_B & 0 & 0 \end{bmatrix} \begin{bmatrix} \delta u_B \\ \delta\tilde{u}_\Pi \\ \delta\lambda \end{bmatrix} = \begin{bmatrix} K_B + B_B^T\lambda - f_B \\ \widetilde{K}_\Pi - \tilde{f}_\Pi \\ B\tilde{u} \end{bmatrix}.$$

Linearized system can be solved using any FETI-DP type method.

We consider hybrid FETI-DP/Multigrid variants: inexact (reduced) FETI-DP

Inexact Reduced Nonlinear FETI-DP

Considering the linearized system

$$\begin{bmatrix} DK_{BB} & D\widetilde{K}_{\Pi B}^T & B_B^T \\ D\widetilde{K}_{\Pi B} & D\widetilde{K}_{\Pi\Pi} & 0 \\ B_B & 0 & 0 \end{bmatrix} \begin{bmatrix} \delta u_B \\ \delta \tilde{u}_\Pi \\ \delta\lambda \end{bmatrix} = \begin{bmatrix} K_B + B_B^T\lambda - f_B \\ \widetilde{K}_\Pi - \tilde{f}_\Pi \\ B\tilde{u} \end{bmatrix}$$

we perform an elimination of δu_B, which yields

$$\begin{bmatrix} \widetilde{S}_{\Pi\Pi} & -D\widetilde{K}_{\Pi B} DK_{BB}^{-1} B_B^T \\ -B_B DK_{BB}^{-1} D\widetilde{K}_{\Pi B}^T & -B_B DK_{BB}^{-1} B_B^T \end{bmatrix} \begin{bmatrix} \delta\tilde{u}_\Pi \\ \delta\lambda \end{bmatrix} = \text{r.h.s.} \tag{3}$$

with $\widetilde{S}_{\Pi\Pi} := D\widetilde{K}_{\Pi\Pi} - D\widetilde{K}_{\Pi B} DK_{BB}^{-1} D\widetilde{K}_{\Pi B}^T$.

Exact solution of $\widetilde{S}_{\Pi\Pi}$ not necessary. Solution of coarse problem is moved to the preconditioner $\Rightarrow$ Inexact solution possible..

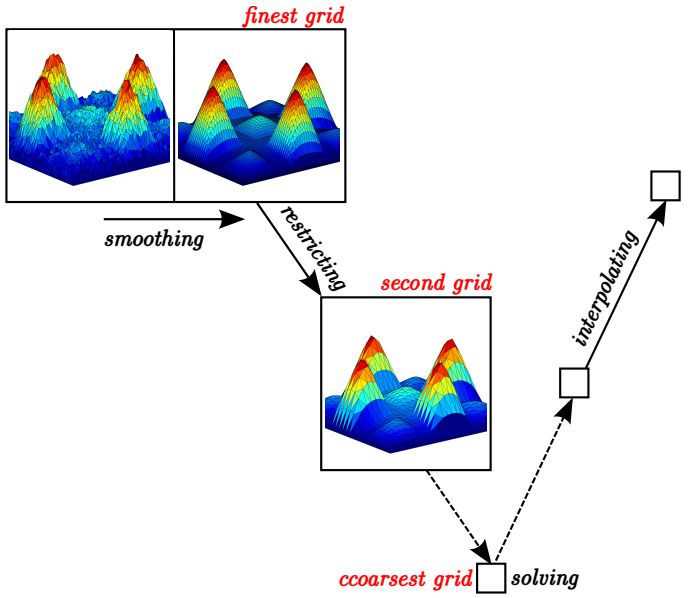
See **Klawonn, Lanser, Rheinbach (SISC, 2015)** for details.

Inexact Reduced Nonlinear FETI-DP

We solve (3) **iteratively** (GMRES) using the block-triangular preconditioner

$$\hat{\mathcal{B}}_{r,L}^{-1} = \begin{bmatrix} \hat{S}_{\Pi\Pi}^{-1} & 0 \\ -M^{-1} B_B D K_{BB}^{-1} D \widetilde{K}_{\Pi B}^T \hat{S}_{\Pi\Pi}^{-1} & -M^{-1} \end{bmatrix}$$

- M^{-1}: one of the standard FETI-DP preconditioners
- $\hat{S}_{\Pi\Pi}^{-1}$: some cycles of an AMG (algebraic multigrid) method, applied to $\widetilde{S}_{\Pi\Pi}$.
- If $\hat{S}_{\Pi\Pi}^{-1}$ is a good preconditioner of $\widetilde{S}_{\Pi\Pi}$, inexact reduced FETI-DP has convergence bounds of the same quality as classical FETI-DP.



One V-cycle of an AMG method.

See **Klawonn, Rheinbach (IJNME 2007, ZAMM 2010)** for details.

Inexact Nonlinear FETI-DP

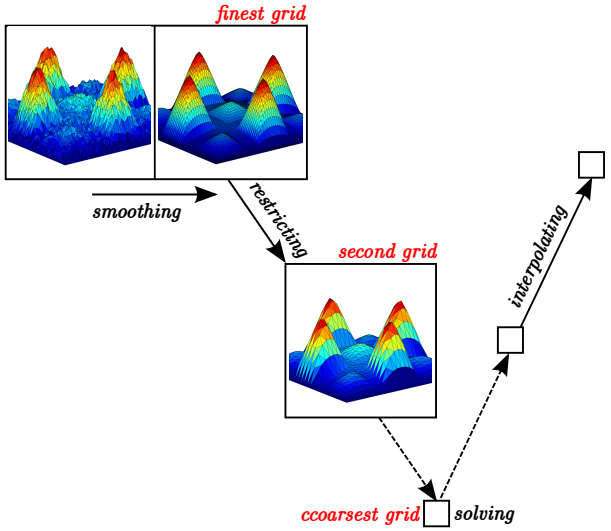
We solve the linearized system

$$\begin{bmatrix} D\widetilde{K} & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \delta\tilde{u} \\ \delta\lambda \end{bmatrix} = \begin{bmatrix} \widetilde{K} + B^T\lambda - \tilde{f} \\ B\tilde{u} \end{bmatrix} \tag{4}$$

iteratively (GMRES) using the block-triangular preconditioner

$$\hat{\mathcal{B}}_L^{-1} = \begin{bmatrix} \hat{K}^{-1} & 0 \\ -M^{-1}B\hat{K}^{-1} & -M^{-1} \end{bmatrix}$$

- $\hat{K}^{-1}$: some cycles of an AMG (algebraic multigrid) method, applied to $D\widetilde{K}$.
- If $\hat{K}^{-1}$ is a good preconditioner of $D\widetilde{K}$, inexact FETI-DP has convergence bounds of the same quality as classical FETI-DP.



One V-cycle of an AMG method.

Inexact Nonlinear FETI-DP

We present two different choices for M^{-1}.

Standard Dirichlet preconditioner:

$$M^{-1} := M^{-1}_{\mathrm{FETI_D}} := \sum_{i=1}^{N} B^{(i)}_{\Delta,D}\, S^{(i)}_{\Delta\Delta}\, B^{(i)T}_{\Delta,D},$$

where $S^{(i)}_{\Delta\Delta} := DK^{(i)}_{\Delta\Delta} - DK^{(i)}_{\Delta I} \left(DK^{(i)}_{II}\right)^{-1} DK^{(i)}_{I\Delta}$ is the Schur complement of the tangential matrix on the interface of subdomain Ω_i. A sparse direct solver is used for $\left(DK^{(i)}_{II}\right)^{-1}$.

Preconditioner without sparse direct solvers:

$$M^{-1} := M^{-1}_{\mathrm{FETI_{D/AMG}}},$$

where $\left(DK^{(i)}_{II}\right)^{-1}$ in M_{FETI_D} is replaced by some applications of sequential AMG to $DK^{(i)}_{II}$.

Implementation Remarks

- **Parallelization Strategy:** MPI based
- Nonlinear FETI-DP is written in C/C++ using **PETSc, Umfpack, MUMPS, PARDISO, BoomerAMG**
- Efficient direct solver packages for local FETI-DP subdomain problems **(Umfpack or MUMPS)**
- If available, the thread parallel direct solver **PARDISO** can also be used for all local FETI-DP subdomain problems
- Parallel AMG implementation **BoomerAMG** is used as a preconditioner for the global FETI-DP coarse problem $\widetilde{S}_{\Pi\Pi}$

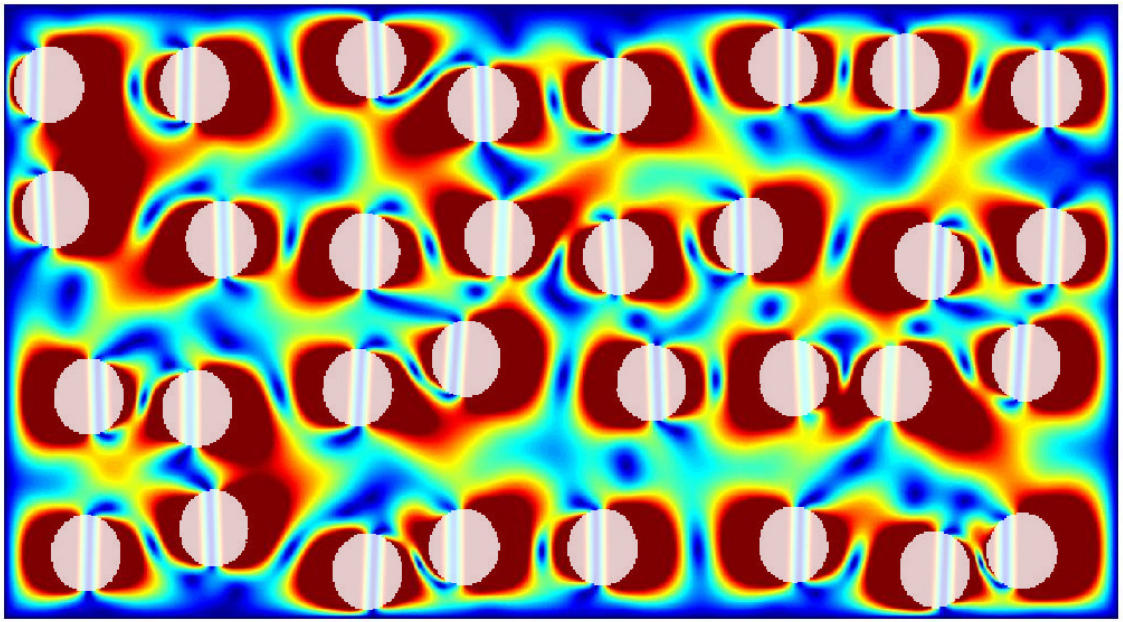
Nonlinear Domain Decomposition

Nonlinear FETI-DP and Nonlinear BDDC: Klawonn, Lanser, Rheinbach (2012, 2013, 2014, 2015) **ASPIN:** Cai, Keyes 2002; Cai, Keyes, Marcinkowski 2002; Hwang, Cai 2005, 2007; Groß, Krause 2010,13; **MSPIN:** Keyes, Liu, 2015 **Nonlinear Neumann-Neumann:** Bordeu, Boucard, Gosselet 2009; **Nonlinear FETI-1:** Pebrel, Rey, Gosselet 2008; **Other DD work reversing linearization and decomposition:** Ganis, Juntunen, Pencheva, Wheeler, Yotov 2014; Ganis, Kumar, Pencheva, Wheeler, Yotov 2014

Model Problem I

- Nonlinear hyperelastic material model: Neo-Hooke
- Heterogeneous material with stiff inclusions ($E = 210\,000$, $\nu = 0.3$) and soft matrix material ($E = 210$, $\nu = 0.3$)
- Deformation is applied on boundary: $F = \begin{bmatrix} 1.1 & 0 \\ 0 & 1 \end{bmatrix}$

Solution with 32 inclusions (white circles) - Visualization of local displacements

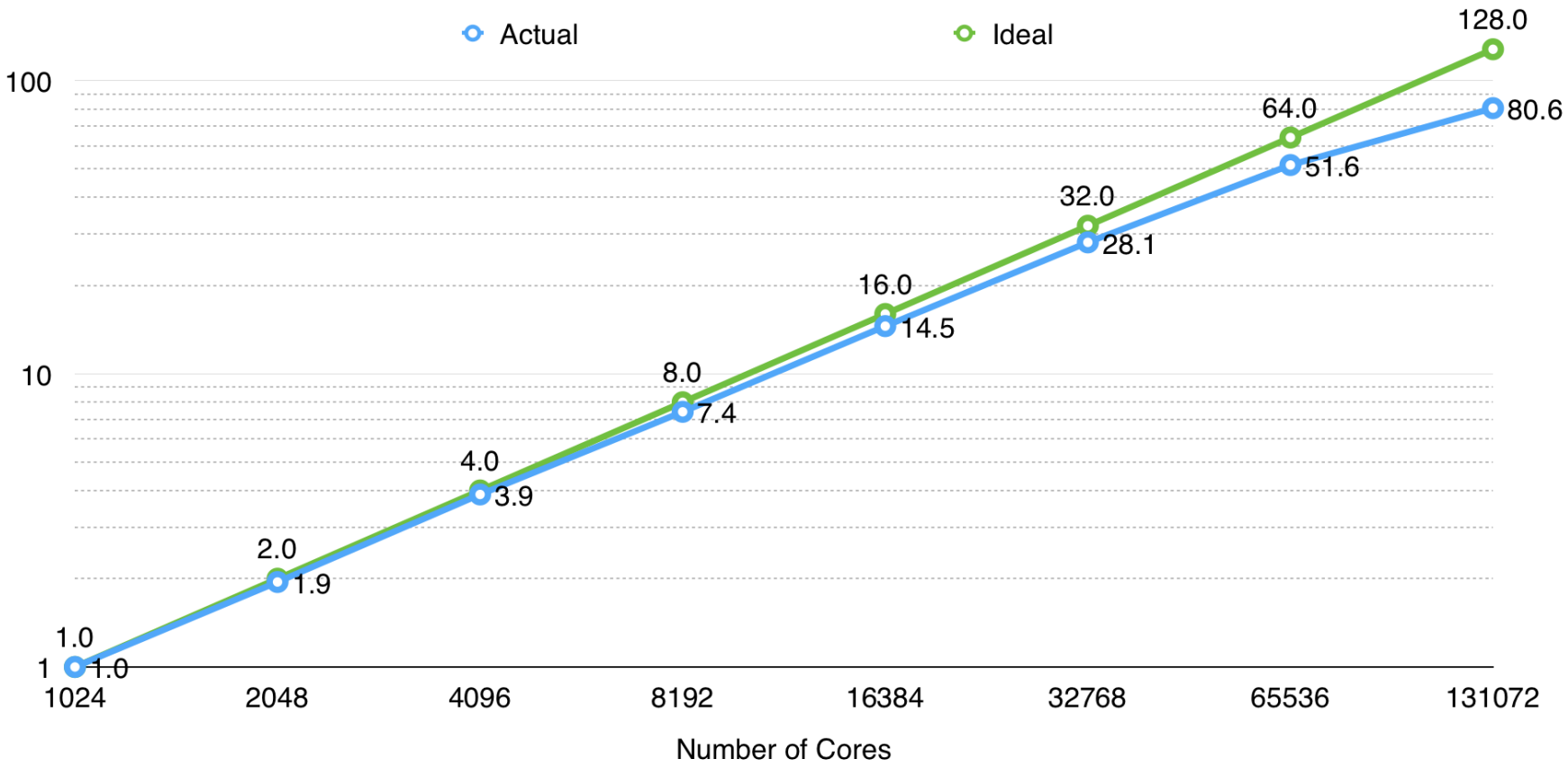


Inexact Reduced Nonlinear-FETI-DP - Strong Scaling

Cores	Subdomains	Problem Size	Execution Time	Actual Speedup	Ideal Speedup	Parallel Effic.
1 024	131 072	419 471 361	3 365.1s	1.0	1	100%
2 048	131 072	419 471 361	1 726.4s	1.9	2	97%
4 096	131 072	419 471 361	868.0s	3.9	4	97%
8 192	131 072	419 471 361	453.5s	7.4	8	93%
16 384	131 072	419 471 361	231.4s	14.6	16	91%
32 768	131 072	419 471 361	119.8s	28.1	32	88%
65 536	131 072	419 471 361	64.3s	51.6	64	81%
131 072	131 072	419 471 361	41.7s	80.6	128	63%

Software / Machine: Vulcan BlueGene/Q at Lawrence Livermore National Laboratory; Using UMFPACK, PETSc 3.4.3 and BoomerAMG from hypre-2.9.4a package; Compiled with IBM compiler. **Problem:** 2D nonlinear hyperelasticity (Neo-Hooke); stiff circular inclusions in soft material; discretized with piecewise quadratic finite elements. **Solver:** Inexact reduced Nonlinear-FETI-DP. Published in Klawonn, Lanser, Rheinbach, SISC 2015.

Inexact Reduced Nonlinear-FETI-DP - Strong Scaling



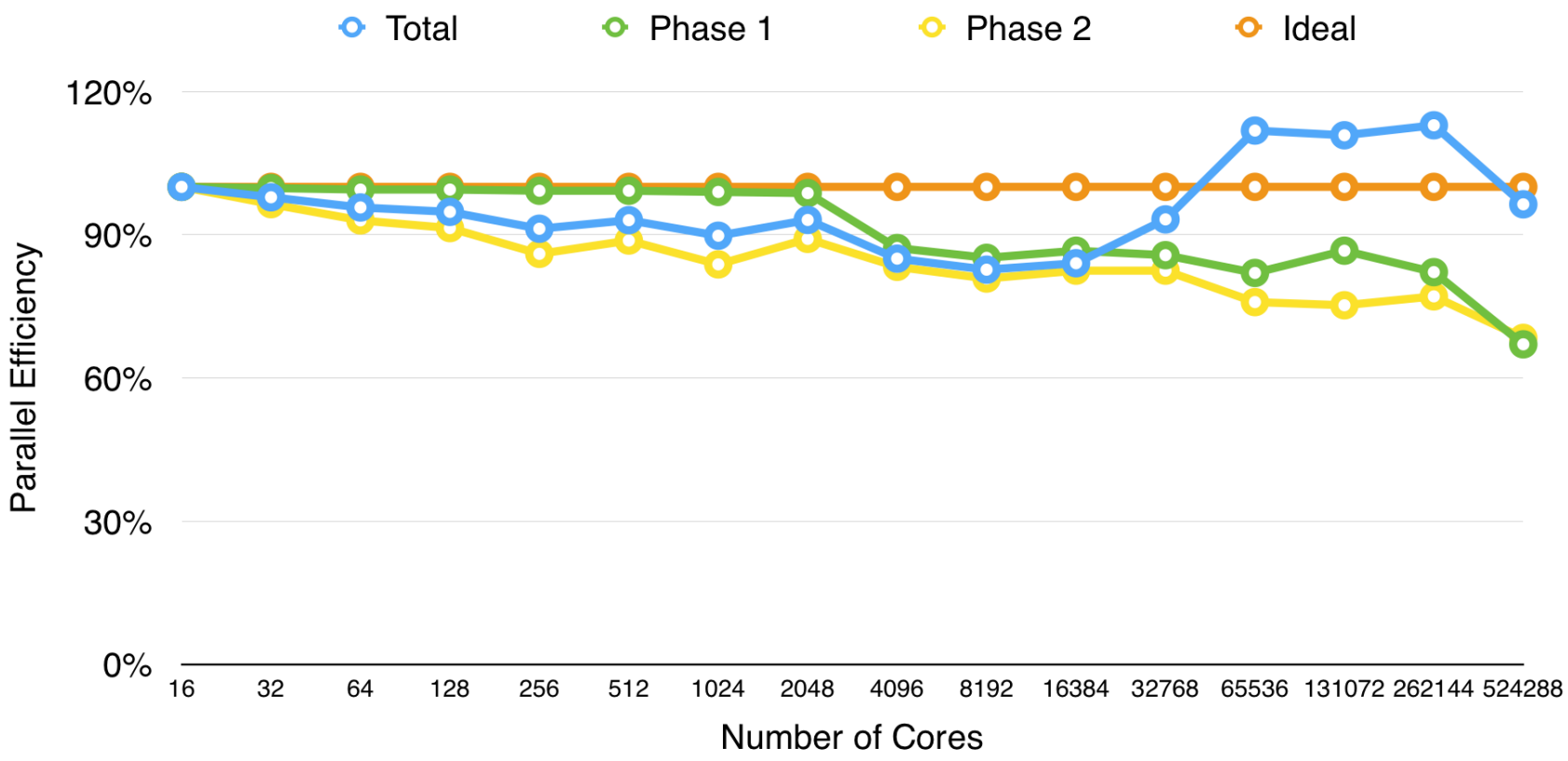
Published in Klawonn, Lanser, Rheinbach, SISC 2015.

Inexact Reduced Nonlinear-FETI-DP - Weak Scaling

Cores	Problem Size	Phase 1 Time / Newton	Phase 2 Time / Newton	Krylov Iter	Total Time	Parallel Efficiency
16	1.3M	158.7s / 4	205.3s / 3	83	**364.0s**	100%
64	5.1M	159.5s /4	220.9s / 3	109	**380.4s**	96%
256	20M	160.1s / 4	238.9s / 3	135	**399.0s**	91%
1 024	82M	160.3s / 4	245.2s / 3	136	**405.5s**	90%
4 096	328M	182.0s / 4	246.5s / 3	110	**428.4s**	85%
8 192	655M	186.4s / 4	254.0s / 3	114	**440.4s**	83%
16 384	1 311M	137.3s / 4	249.0s / 3	110	**433.3s**	84%
32 768	2 622M	138.9s / 4	251.7s / 3	111	**390.6s**	93%
65 536	5 243M	145.3s / 4	180.3s / **2**	85	**325.6s**	112%
131 072	10 486M	147.5s / **3**	182.0s / **2**	84	**329.5s**	110%
262 144	20 972M	144.9s / **3**	177.5s / **2**	83	**322.4s**	113%
524 288	41 944M	177.6s / **3**	200.2s / **2**	82	**377.8s**	96%

Software / machine: Mira BlueGene/Q at Argonne National Laboratory; Using MUMPS, PETSc 3.5.2 and BoomerAMG from hypre-2.9.1a package; Compiled with IBM compiler. **Problem:** 2D nonlinear hyperelasticity (Neo-Hooke); stiff circular inclusions in soft material; discretized with piecewise quadratic finite elements. **Solver:** Inexact reduced Nonlinear-FETI-DP. Published in Klawonn, Lanser, Rheinbach, SISC 2015.

Inexact Reduced Nonlinear-FETI-DP - Weak Scaling

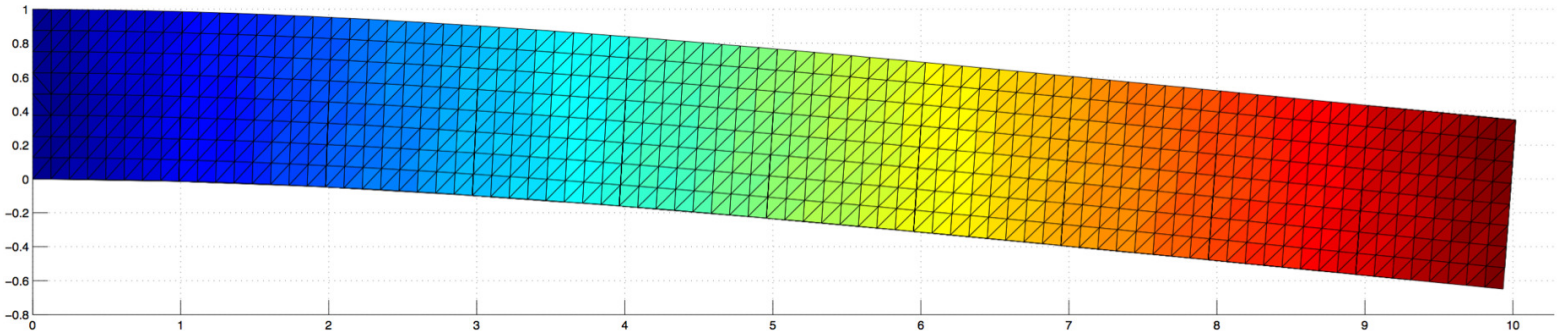


Published in Klawonn, Lanser, Rheinbach, SISC 2015.

Model Problem II

- Nonlinear hyperelastic material model: Neo-Hooke
- Homogeneous material ($E = 210$, $\nu = 0.3$)
- Rectangular domain with aspect ratio 8:1, fixed on one of the short edges
- Volume force in vertical direction

Solution of a Small Example



Inexact Nonlinear-FETI-DP

# MPI ranks	D.o.f.	M^{-1}	It.	Time to Solution	Time Setup Saddlepoint system	Time GMRES
32	643 602	$M^{-1}_{\mathrm{FETI_D}}$	66	53.4s	5.7s	21.0s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	70	56.7s	5.7s	31.5s
512	10 254 402	$M^{-1}_{\mathrm{FETI_D}}$	57	55.2s	6.0s	18.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	66	58.5s	6.1s	30.2s
8 192	163 897 602	$M^{-1}_{\mathrm{FETI_D}}$	52	55.9s	6.4s	17.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	64	59.5s	6.4s	29.5s
131 072	2 621 670 402	$M^{-1}_{\mathrm{FETI_D}}$	44	60.4s	8.6s	15.0s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	61	65.7s	8.5s	28.5s
524 288	10 486 220 802	$M^{-1}_{\mathrm{FETI_D}}$	47	86.6s	17.6s	17.1s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	66	94.0s	17.8s	32.5s

Software / Machine: JUQUEEN BlueGene/Q at JSC Jülich; Using MUMPS, PETSc 3.6.2 and BoomerAMG from hypre-2.10.1 package; Compiled with IBM compiler; discretized with piecewise quadratic finite elements. **Solver:** Inexact Nonlinear-FETI-DP. **AMG:** GM approach (BoomerAMG).

Conclusion

- Highly scalable combinations of domain decomposition and AMG
- Strong and weak scalability for heterogeneous and nonlinear elasticity
- Scalable and robust FETI-DP/AMG method without sparse direct solvers

Acknowledgement

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- The use of **Vulcan** at Lawrence Livermore National Laboratory is gratefully acknowledged.
- Support is gratefully acknowledged by Deutsche Forschungsgemeinschaft (DFG) within the priority program SPP 1648 Software for Exascale Computing

Related Publications

[1] Allison H. Baker, Axel Klawonn, Tzanio Kolev, Martin Lanser, Oliver Rheinbach, and Ulrike Meier Yang. Scalability of classical algebraic multigrid for elasticity to half a million parallel tasks. 2015. Submitted 11/2015 to Lect. Notes Comput. Sci. Eng. TUBAF Preprint: 2015-14, http://tu-freiberg.de/fakult1/forschung/preprints.

[2] Daniel Balzani, Ashutosh Gandhi, Axel Klawonn, Martin Lanser, Oliver Rheinbach, and Jörg Schröder. One-way and fully-coupled FE^2 methods for heterogeneous elasticity and plasticity problems: Parallel scalability and an application to thermo-elastoplasticity of dual-phase steels. 2015. Submitted 11/2015 to Lect. Notes Comput. Sci. Eng. TUBAF Preprint: 2015-14, http://tu-freiberg.de/fakult1/forschung/preprints.

[3] Axel Klawonn, Martin Lanser, and Oliver Rheinbach. FE^2TI: Computational scale bridging for dual-phase steels. 2015. Accepted to ParCo 2015. TUBAF Preprint: 2015-12, http://tu-freiberg.de/fakult1/forschung/preprints.

[4] Axel Klawonn, Martin Lanser, and Oliver Rheinbach. A highly scalable implementation of inexact nonlinear FETI-DP without sparse direct solvers. 2015. Accepted to the Proceedings of the ENUMATH Conference 2015. TUBAF Preprint: 2015-17, http://tu-freiberg.de/fakult1/forschung/preprints.

[5] Axel Klawonn, Martin Lanser, and Oliver Rheinbach. A highly scalable implementation of inexact nonlinear FETI-DP without sparse direct solvers. December 2015. Accepted for publication in the proceedings of the European Conference on Numerical Mathematics – ENUMATH2015, Lect. Notes Comput. Sci. Eng. TUBAF Preprint: 2015-17, http://tu-freiberg.de/fakult1/forschung/preprints.

[6] Axel Klawonn, Martin Lanser, and Oliver Rheinbach. Towards extremely scalable nonlinear domain decomposition methods for elliptic partial differential equations. *SIAM J. Sci. Comput.*, 37(6):C667–C696, December 2015.

[7] Axel Klawonn, Martin Lanser, Oliver Rheinbach, Holger Stengel, and Gerhard Wellein. Hybrid MPI/OpenMP parallelization in FETI-DP methods. In Miriam Mehl, Manfred Bischoff, and Michael Schfer, editors, *Recent Trends in Computational Engineering - CE2014*, volume 105 of *Lecture Notes in Computational Science and Engineering*, pages 67–84. Springer International Publishing, 2015.

[8] Oliver Rheinbach. Homogenisierung im Höchstleistungsrechner. *Acamonta - Zeitschrift für Freunde und Förderer der Technischen Universität Bergakademie Freiberg*, 22:40–43, 2015.