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FE²TI: Computational Scale Bridging for Dual-Phase Steels

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Abstract. A scale bridging approach combining the FE² method with parallel domain decomposition (FE²TI) is presented. The FE²TI approach is used in the project “EXASTEEL - Bridging Scales for Multiphase Steels” (within the German priority program “Software for Exascale Computing - SPPEXA”) for the simulation of modern dual-phase steels. This approach incorporates phenomena on the microscale into the macroscopic problem by solving many independent microscopic problems on representative volume elements (RVEs). The results on the RVEs replace a phenomenological material law on the macroscale. In order to bring large micro-macro simulations to modern supercomputers, in the FE²TI approach a highly scalable implementation of the inexact reduced FETI-DP (Finite Element Tearing and Interconnecting - Dual Primal) domain decomposition method (scalable up to 786 432 Mira BlueGene/Q cores) is used as a solver on the RVEs. Weak scalability results for the FE²TI method are presented, filling the complete JUQUEEN at JSC Jülich (458 752 cores) and the complete Mira at Argonne National Laboratory (786 432 cores).

Keywords. Computational Scale Bridging, Domain Decomposition, FETI-DP, FE²

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Introduction

We are concerned with the computational simulation of advanced high strength steels, incorporating phase transformation phenomena at the microscale. The project “EXASTEEL - Bridging Scales for Multiphase Steels” is part of the German priority program (DFG-Schwerpunktprogramm 1648) SPPEXA (Software for Exascale Computing) and one of its goals is bringing computational scale bridging methods such as the FE² method to recent supercomputers. The FE² method, see, e.g., [1,2,3,4,5], is a computational micro-macro scale bridging approach directly incorporating micromechanics into macroscopic simulations. In this approach, a microscopic boundary value problem based on the definition of a representative volume element (RVE) is solved at each Gauß integration point of a macroscopic finite element problem. Then, volumetric av-

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erages of microscopic stress distributions are returned to the macroscopic level, which replaces a phenomenological material law at the macro scale. The microscopic problems are only coupled through the macroscopic problem; see Figures 1 and 2. On the RVEs nonlinear implicit structural mechanics problems have to be solved. We are applying the inexact reduced FETI-DP (Finite Element Tearing and Interconnecting) method as a solver on the RVEs. Nonoverlapping domain decomposition methods of the FETI type [6,7,8,9,10,11,12,13,14,15] are well established solution methods in implicit structural mechanics. A structural simulation using a FETI-DP algorithm was awarded a Gordon Bell prize already in 2002 using 4 000 processors of the then second fastest supercomputer of the world. However, the classical FETI-DP method does not scale well beyond 10K processor cores. Inexact FETI-DP methods [16], have shown a much better parallel scalability, and scalability for 65 536 cores was shown during the 2008 JUGENE scaling workshop in Jülich [17,13]. Recently, nonlinear FETI-DP and BDDC methods [18,19,20] with improved concurrency were introduced. In these methods, the nonlinear problem is decomposed into concurrent subproblems before linearization. This is opposed to standard Newton-Krylov approaches where the problem is first linearized and then decomposed. Hybrid parallelization in our context was discussed in [21]. Nonlinear nonoverlapping domain decomposition is not new. It was used, e.g., in multiphysics and fluid-structure-interaction as a coupling method in the case of a small number of subdomains. Only recently, it has attracted interest as a scalable solver approach [22,23,18,19,20]. The ASPIN method [24] is a related nonlinear overlapping domain decomposition approach as a solver.

We refer to the combination of the FE^2 scale bridging method with a FETI-DP method on each RVE as a FE^2TI method. For our FE^2 method, as a solver on the RVEs, we use a Newton-Krylov-irFETI-DP method. For the first time weak scalability results for the FE^2TI method for the complete Mira BlueGene/Q (rank 5 in the current TOP500 list 06/2015, Argonne National Laboratory) is presented and also scalability for the complete JUQUEEN BlueGene/Q (rank 9 in current TOP500 list 06/2015, Jülich Supercomputing Centre). This current paper is an extended version of the technical report [25] on JUQUEEN scaling results. The results on Mira have been obtained later and have benefited from the experience gained on JUQUEEN.

1. The FE^2TI Method

1.1. Problem Statement and Algorithmic Description

We provide an algorithmic overview of the FE^2 method using FETI-DP on the RVEs in Figure 3. We proceed by discussing the steps in Figure 3. The FE^2 method considers a macroscopic problem and many independent microscopic finite element problems. The undeformed macroscopic body $\bar{\mathcal{B}}_0$ can be discretized with relatively large finite elements neglecting the microscopic structure. We are interested in a macroscopic deformation gradient \bar{F} and a macroscopic first Piola-Kirchhoff stress tensor \bar{P} fulfilling the balance of momentum

$$-\int_{\bar{\mathcal{B}}_0} \delta \bar{x} \cdot (\text{Div } \bar{P}(\bar{F}) + \bar{f}) dV = 0$$

under suitable boundary conditions, an external load \bar{f} , and with a variational function $\delta\bar{x}$. In order to incorporate the microstructure, a nonlinear boundary value problem resolving the microstructure is then considered in each Gauß interpolation point of the macroscopic problem.

These problems replace a phenomenological material law deriving the stress \bar{P} directly from the deformation \bar{F} . The geometry of the microscopic problem has to represent the heterogeneity of the material effectively and is derived from the definition of a representative volume element (RVE) \mathcal{B}_0 . Applying boundary constraints derived from the deformation gradient \bar{F} , we solve the microscopic problems using an inexact reduced FETI-DP type domain decomposition method; “1.” and “2.” in Figure 3. After convergence of the microscopic problem, the macroscopic stress \bar{P} in the corresponding Gauß integration point is given as the volumetric average of the microscopic stresses $P(F)$; “3.” in Figure 3. Let us remark that we assume a phenomenological law $P(F)$ on the microscale, as, e.g., a Neo-Hookean hyperelasticity model or a J2 elasticity-plasticity model. Since high peaks in the stress can lead to material failure and are typically a microscopic phenomenon, the microscopic stresses $P(F)$ have to be considered in order to predict material failure. In order to solve the macroscopic problem, the discrete macroscopic tangent modulus $\bar{\mathbb{A}}^h$ has to be computed, which can also be performed by averaging microscopic quantities; “4.” in Figure 3. The term $L^T(DK)^{-1}L$ in “4.” of Figure 3 requires the solution for nine right hand sides on the micro scale, i.e., we have nine additional microscopic FETI-DP solves. Here, DK is the tangential matrix of the microscopic problem in the stationary point and L contains nine different right hand sides; see [2] for more details. Using $\bar{\mathbb{A}}^h$ and \bar{P}^h , the macroscopic problem can be assembled and solved; “5.”, “6.”, and “7.” in Figure 3.

Let us remark that Figure 3 describes a single macroscopic load step. The total deformation \bar{F} may only be reached using many incremental load steps. In each such load step, a macroscopic Newton iteration is performed and in each macroscopic Newton step a nonlinear microscopic boundary value problem is solved in each macroscopic Gauß integration point.

1.2. Granularity and Load Balancing

Let us finally provide a short description of the parallelism of the FE2TI algorithm. First, we distribute the RVEs. Each RVE is assigned to its own MPI communicator obtained by an `MPI.Comm.split`. Then, the RVEs are decomposed geometrically into nonoverlapping FETI-DP subdomains. Each subdomain is assigned to one MPI rank of the RVE subcommunicator. In order to obtain an optimal load balance and properly distributed data, the sizes of all subdomains have to be similar and each MPI rank should handle the same number of subdomains. Most of the FETI-DP matrices and data structures can be created and saved locally, only using the mesh information related to a subdomain. Parallel structures, as the FETI-DP coarse space, are implemented using the parallel matrix and vector classes provided by PETSc. Thus, these structures are distributed linearly to all MPI ranks of the RVE subcommunicator. A detailed description of the parallel implementation of inexact FETI-DP methods can be found in [26].

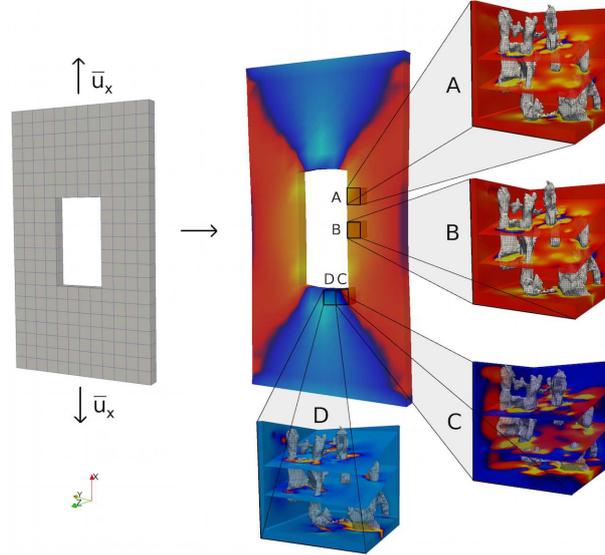


Figure 1. FE2TI computation with 1 792 RVEs and real micro structure; cf. Section 2.3. The computation was performed on all 28 racks of JUQUEEN. Left: Undeformed rectangular plate with a hole discretized by 224 Q1 finite elements with 8 Gauß points each. Right: Visualization of the von Mises stresses of the deformed macroscopic problem and four exemplary RVEs in different Gauß points (A,B,C,D). The stress peaks in the microstructures are 5-7 times higher than the peaks in the macroscopic problem.

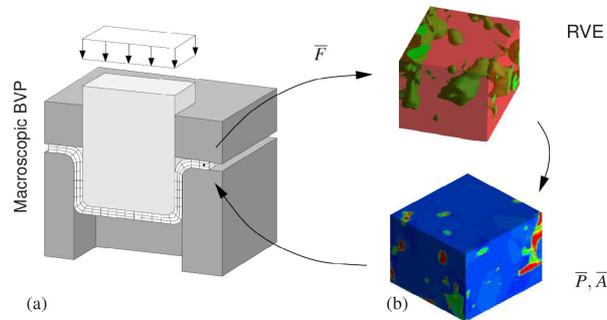


Figure 2. FE² approach with (a) macroscopic boundary value problem (BVP) and (b) microscopic BVP on an RVE. In the FE² computational scale bridging method, in each macroscopic Gauß point a microscopic problem is solved.

1.3. Implementation

We have implemented the FE² method using PETSc 3.5.2 [27] using C/C++ and MPI and MPI/OpenMP. Furthermore, we rely on MUMPS [28,29], UMFPACK [30] or PAR-DISO [31] for sequential (or parallel) direct solves. Note that on the BlueGene/Q, when linked to the ESSL and for our setting with nine right hand sides on the micro structure, UMFPACK and MUMPS showed very similar performance. This is opposed to our experience on other architectures, where MUMPS often showed a better performance. The algebraic multigrid solver BoomerAMG [32] from the hypre [33] package is used in our

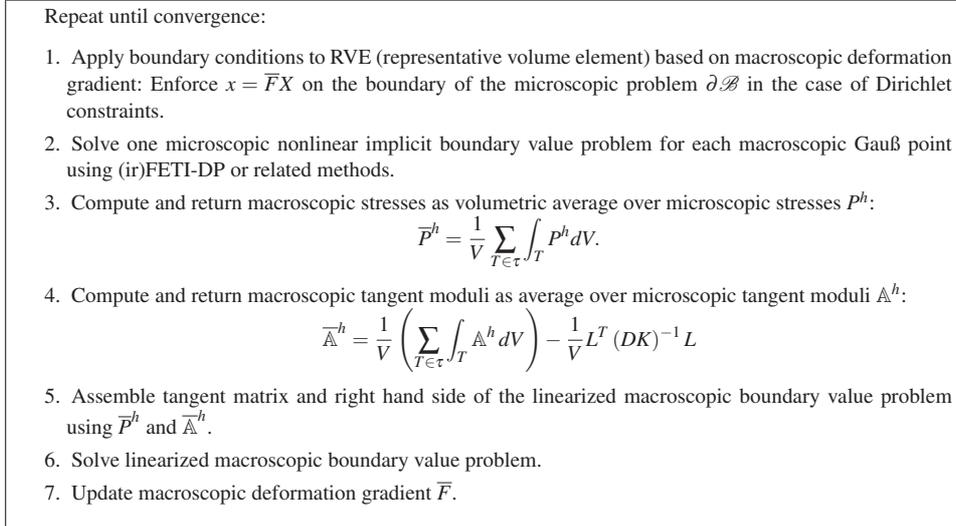


Figure 3. Algorithmic description of the FE²TI approach. Overlined letters denote macroscopic quantities.

inexact reduced FETI-DP methods as a preconditioner of the FETI-DP coarse problem. All packages are interfaced through PETSc. On Blue Gene/Q, the software environment is compiled using the IBM XL C/C++ compilers to profit from auto vectorization. Since the lion's share of the runtime is spent in IBM's ESSL library when using UMFPACK for all direct solves, the effect of (additional) auto vectorization is limited. The macroscopic problem is discretized using piecewise trilinear brick elements (Q1) in three dimensions.

2. Numerical Results

The FE²TI computational scale bridging software is member of the High-Q-Club² after having scaled to the complete 28 racks of the JUQUEEN BlueGene/Q in Jülich in 2015; see the JUQUEEN scaling report [25]. FE²TI also scales to the complete 48 BlueGene/Q racks of Mira. The scaling runs presented here always consist of one macroscopic load step using a heterogenous nonlinear hyperelasticity material on the microscale. In our application, we are also interested in plastification on the RVEs. We will perform corresponding numerical experiments in the near future.

2.1. Scalability of the Method on the JUQUEEN Supercomputer (JSC, Jülich)

We present our scaling results for the computational scale bridging in 2D and 3D. Most of the scaling results for the complete JUQUEEN machine were achieved on the Workshop on "Extreme Scaling on JUQUEEN" and collected in the technical report [25]. This paper builds on this report. Details on the FETI-DP iterative solver algorithm and successive improvements of the solver to enhance its scalability on JUQUEEN and other supercomputers are submitted as [26].

²http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/FE2TI/_node.html

We first scale up the size of the macroscopic problem while keeping the size of the microscopic RVEs fixed. We also keep the number of FETI-DP subdomains for each RVE fixed and use one MPI rank per FETI-DP subdomain. As we increase the number of processor cores in proportion to the problem size (weak scalability), in the best case, for a parallel efficiency of 100%, we would expect a constant time to solution. In Tables 1 and 2, we present the weak scalability for 2D and 3D; we use one MPI rank for each BlueGene/Q processor core and threading with 4 OpenMP threads. The baseline for our parallel efficiency is the smallest meaningful macroscopic problem, i.e., with 8 Gauß points in 2D and 16 Gauß points in 3D. A parallel efficiency of approximately 98% is achieved in Tables 1 and 2. These results confirm the assumed good weak scalability behavior of the method and the potential to scale to even larger machines. Thus, the FE²TI approach is suitable and efficient for large multiscale simulations.

In our implementation, we use `MPI_Comm_split` to create subcommunicators for the computations on the RVEs. We use the environment variable `PAMID_COLLECTIVES_MEMORY_OPTIMIZED=1` to keep the time for the communicator split short. In our computations the resulting timings for the communicator split was below 2 seconds. In Tables 1 and 2, the number of subdomains for each RVE, i.e., 256 in 2D and 512 in 3D, is still small. In Table 3, starting from the largest problem in Table 1, the size of the RVEs is increased by a factor of 4.

Next, we disable OpenMP threading and consider the effect of oversubscription using pure MPI. In Table 4, we show weak scaling but using oversubscription with up to 4 MPI ranks for each BlueGene/Q processor core. In the latter case, only 256 MB are available for each MPI rank. We use 16, 32, and 64 MPI ranks per node and the RVE size is kept constant, i.e., the total problem size is increased by a factor of 4. We, of course, cannot expect perfect scalability in this situation. But we still see that acceptable scalability is obtained when scaling from a total of 458752 MPI ranks to 917504 MPI ranks, i.e., the total time to solution is 266.47s instead of $2 \cdot 215.41s = 430.82s$. Using 1835008 MPI ranks only gives minor additional savings. From these results, when we are not using OpenMP threading, we now use 32 MPI ranks per node as a default. Of course, we then have to respect the memory constraint of 512 MB.

We see that the algorithmic approach of solving the macroscopic FE² problem fully redundantly is currently sufficient, given the three level structure of the algorithm with the very aggressive coarsening on the third level: In the largest case on JUQUEEN in Table 4, we have 1.8 million subdomains, 3 584 concurrent FETI-DP coarse problems, and a macroscopic problem of size 3 051. Nevertheless, we may move to a parallel solve of the macro problem in the future.

2.2. Scalability of the Method on the Mira Supercomputer (ALCF, Argonne Nat. Lab.)

We present our scaling results for the FE²TI method in 3D. During the Mira Bootcamp 2015 we have achieved weak scalability up to the full Mira supercomputer, i.e., 786432 cores using 1.5 million MPI ranks; see Table 5. These results have not been presented elsewhere. In Table 5, weak scalability in 3D is presented where the baseline for the parallel efficiency is, again, the smallest meaningful macroscopic problem, i.e., using 16 Gauß points in 3D. A parallel efficiency of approximately 96.9% is achieved, which is remarkable. These results could only be achieved by building in the experience previously gained on the JUQUEEN supercomputer and show the potential of the method beyond today's supercomputer.

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Table 1. Scaling up the macro problem: FE² in 2D using FETI-DP on each RVE; heterogeneous hyperelasticity; P1 finite elements macro, P2 finite elements micro; 5.1 million d.o.f. on each RVE; 256 subdomains for each RVE; 4 OpenMP threads per MPI rank.

FE ² TI in 2D (Weak scaling; JUQUEEN)				
Cores	MPI-ranks	#RVEs	Time to Solution	
2 048	2 048	8	158.47s	100.0%
4 096	4 096	16	159.03s	99.6%
8 192	8 192	32	159.27s	99.5%
16 384	16 384	64	159.32s	99.5%
32 768	32 768	128	159.58s	99.3%
65 536	65 536	256	159.68s	99.2%
131 072	131 072	512	159.99s	99.1%
262 144	262 144	1 024	160.62s	98.7%
393 216	393 216	1 536	161.41s	98.2%
458 752	458 752	1 792	161.78s	98.0%

Table 2. Scaling up the macro problem (small RVEs): FE² in 3D using FETI-DP on each RVE. Time for a single load step of heterogeneous hyperelasticity; Q1 finite elements macro, P2 finite elements micro; 1.6 million d.o.f. on each RVE; 512 subdomains for each RVE; 4 OpenMP threads per MPI-rank.

FE ² TI in 3D (Weak scaling; JUQUEEN)				
Cores	MPI-ranks	#RVEs	Time to Solution	
8 192	8 192	16	184.86s	100.0%
16 384	16 384	32	185.09s	99.9%
32 768	32 768	64	185.61s	99.6%
65 536	65 536	128	185.72s	99.5%
131 072	131 072	256	186.43s	99.2%
262 144	262 144	512	186.61s	99.1%
393 216	393 216	768	187.32s	98.7%
458 752	458 752	896	187.65s	98.5%

Table 3. We increase the RVE sizes starting from the largest problem in Table 1; heterogeneous hyperelasticity; P1 finite elements macro, P2 finite elements micro.

FE ² TI in 2D (Increasing RVE sizes; JUQUEEN)					
Cores	MPI-ranks	#RVEs	RVE-size	RVE-size × #RVEs	Time to Solution
458 752	458 752	1 792	5 126 402	9 186 512 384	161.78s
458 752	458 752	1 792	7 380 482	13 225 823 744	248.19s
458 752	458 752	1 792	13 117 442	23 506 456 064	483.68s
458 752	458 752	1 792	20 492 802	36 723 101 184	817.06s

Table 4. “Weak scaling-type” efficiency using 16 / 32 / 64 MPI-ranks per node while increasing the problem size proportionally to the number of MPI ranks. FE² in 3D using FETI-DP on each RVE (FE²TI). We use 1 594 323 d.o.f. per RVE and 512 subdomains per RVE.

FE ² TI in 3D (1x, 2x, 4x MPI overcommit; JUQUEEN)					
Cores	ranks per node	MPI-ranks	#RVEs	Time to Solution	
458 752	16	458 752	896	215.41s	100%
458 752	32	917 504	1 792	266.47s	81%
458 752	64	1 835 008	3 584	522.10s	41%

2.3. Production Runs on JUQUEEN

We were able to run for the first time large scale 3D FE² multiscale simulations with 40 load steps using the complete JUQUEEN supercomputer. The total computation used 5

Table 5. Scaling up the macro problem (large RVEs) on Mira using multiple subdomains per core: FE² in 3D using FETI-DP on each RVE. Time for a single load step of heterogeneous hyperelasticity; Q1 finite elements macro, P2 finite elements micro; 12.5 million d.o.f. on each RVE; 4 096 subdomains for each RVE; 1 024 MPI ranks and 512 cores per RVE.

FE ² TI in 3D (Weak scaling; Mira)					
Cores	MPI ranks	#RVEs	Total dof	Time to Solution	
8 192	16 384	16	200M	914.34s	100.0%
16 384	32 768	32	401M	932.96s	98.0%
32 768	65 536	64	801M	932.48s	98.1%
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%

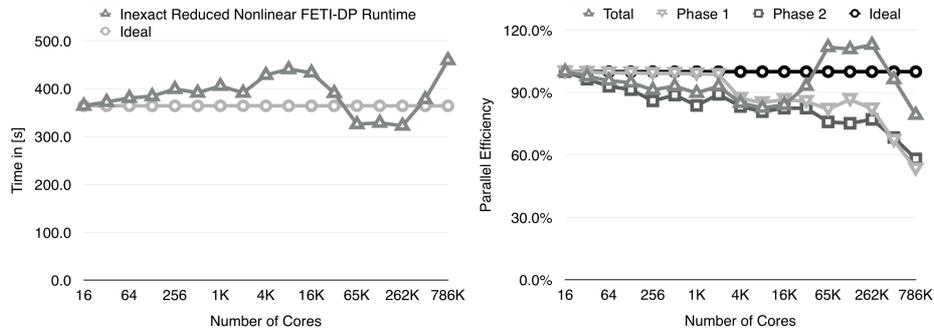


Figure 4. Left: Time to solution of inexact reduced Nonlinear-FETI-DP applied to a heterogeneous 2D Neo-Hooke hyperelasticity problem. Weak scalability from 16 up to 786432 cores on MIRA Blue Gene/Q. The largest problem has 62.9 billion degrees of freedom. **Right:** Parallel Efficiency of the algorithm.

hours on the full 28 racks to compute a deformation of 8%. To the best of our knowledge, no FE² simulations of this size have been carried out before. We confirmed the expected stress concentrations at the microscopic level which are significantly higher than at the macroscopic level; see Figure 1 for a visualization of the stresses.

2.4. Scalability of the Solver on the Microscale - Inexact FETI-DP

We use a FETI-DP method to solve the nonlinear microscopic problems on the RVEs. Substantial effort has been made to obtain good scalability for our FETI-DP methods. Weak scalability results of inexact reduced Nonlinear FETI-DP is presented in Figure 4 for up to 786432 cores of the Mira supercomputer for a model problem. Choosing the total time to solution on 16 cores as a baseline, we achieve a parallel efficiency of 79.3% on 786K cores. Here, we benefit from a decreasing number of Newton steps needed for convergence. Using a different metric to measure the scalability, i.e. the average time per Newton step, we also achieve a good efficiency of more than 53%; see Phase 1 and 2 in Figure 4 (Right). The largest problem has approximately 63 billion unknowns. These results are also part of the submitted publication [26].

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2.5. Conclusion

We performed multiscale simulations using the FE^2 method for the first time at the full scale of the largest supercomputers currently available, both using pure MPI and (limited) hybrid OpenMP/MPI parallelization. This has been achieved by continuously improving the performance and scalability of the FE^2 implementation. Moreover, we have pushed the weak parallel scalability of implicit domain decomposition solvers to over half a million cores making these computations the largest currently known to us for a domain decomposition solver in terms of the number of cores as well as the problem size.

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