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OBJECTIVE MULTISCALE ANALYSIS OF RANDOM HETEROGENEOUS MATERIALS

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Abstract. The multiscale framework presented in [1, 2] is assessed in this contribution for a study of random heterogeneous materials. Results are compared to direct numerical simulations (DNS) and the sensitivity to user-defined parameters such as the domain decomposition type and initial coarse scale resolution is reported. The parallel performance of the implementation is studied for different domain decompositions.

1 INTRODUCTION

Numerical methods employed for the simulation of physical processes are regarded useful for the scientific community when they prove to be robust, computationally affordable and objective with respect to a number of user-defined parameters. This is the case of the finite element (FE) method which proves to be a valuable tool for solving partial differential equations by integrating a weak form of the variational statement on a user-defined support which varies throughout different discretizations. Results of well-posed problems turn to be objective with respect to the discretization, assuming that a minimum FE size is adopted, and are regarded as an approximation of the analytical reference solution.

Computational multiscale techniques demand similar requirements in order to be considered applicable. The multiscale simulation of softening materials that show localized failure patterns is a good example where objectivity is a challenging aspect. Hierarchical multiscale approaches, in which a microstructural representative volume element (RVE)

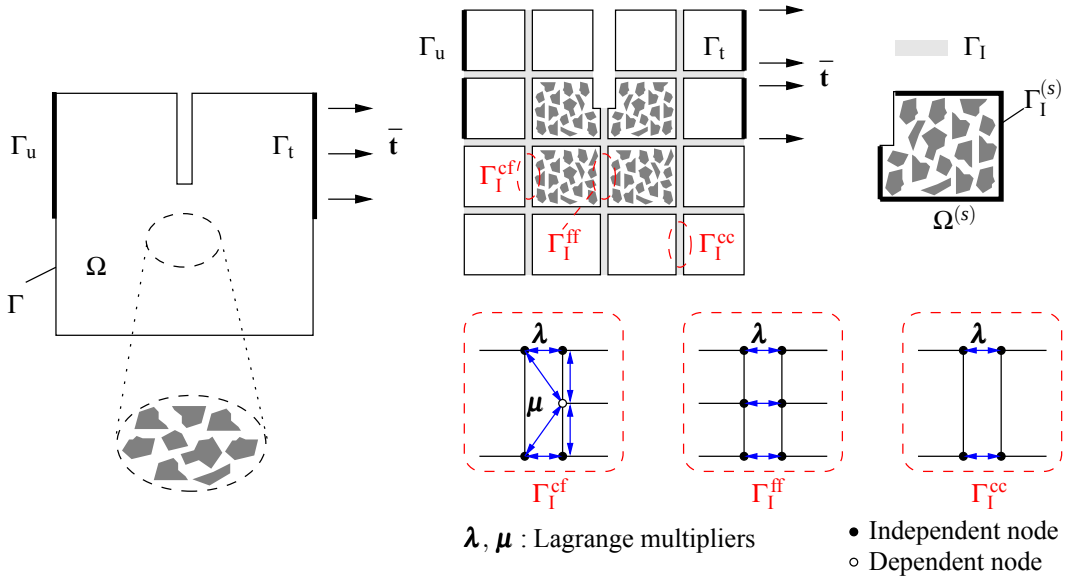

Figure 1: Heterogeneous solid Ω (left). Domain decomposition using a dual connection strategy (right).

is used to compute the constitutive relation at the macroscale, have been recently proposed where the overall result is objective with respect to the RVE size [3, 4, 5, 6, 7]. In concurrent multiscale analysis, the region over which a zoom-in is performed can vary according to user parameters such as the criteria for the coarse-to-fine transition and mesh adaptation [8, 9, 10]. However, an objective response is expected provided that the refined region captures the spread of non-linearity in the material sample. Multiscale approaches based on domain decomposition methods [11, 1, 12] are seen as particular concurrent multiscale techniques where the zoom-in regions are linked to the size and shape of the partitions. Objectivity of the results with respect to these parameters has been shown in [13, 1] for homogeneous analysis. Random heterogeneous material samples are studied in this contribution in order to assess the objectivity of domain decomposition multiscale frameworks.

2 MULTISCALE DOMAIN DECOMPOSITION ANALYSIS

The multiscale approach utilized in this contribution has been presented in [1, 2] and is based on an extension of non-overlapping domain decomposition techniques with different domain resolutions. A short introduction to the adaptive multiscale approach is provided in the remaining of this section.

2.1 Dual formulation of the concurrent multiscale framework

Consider a body Ω with heterogeneous underlying structure and boundary conditions depicted in Figure 1 (left). The variational form of a general equilibrium problem for Ω can be discretized, in a linear context, using standard FE procedures and the resulting

set of equations reads

$$\mathbf{K}\mathbf{u} = \mathbf{f}, \tag{1}$$

where $\mathbf{K}$, $\mathbf{u}$ and $\mathbf{f}$ denote the global stiffness matrix, displacement vector and force vector, respectively.

The body Ω is divided into N_s non-overlapping domains $\Omega^{(s)}$ connected by the interface Γ_I (right part of Figure 1). Coarse (c) and fine (f) material resolutions are handled simultaneously in the computations and the resulting interface satisfies $\Gamma_\mathrm{I} = \Gamma_\mathrm{I}^{\mathrm{cc}} \cup \Gamma_\mathrm{I}^{\mathrm{ff}} \cup \Gamma_\mathrm{I}^{\mathrm{cf}}$, where the superscripts denote coarse-to-coarse mesh connection (cc), fine-to-fine mesh connection (ff) and coarse-to-fine mesh connection (cf). In our approach $\Gamma_\mathrm{I}^{\mathrm{cc}}$ and $\Gamma_\mathrm{I}^{\mathrm{ff}}$ are conforming whereas $\Gamma_\mathrm{I}^{\mathrm{cf}}$ is non-conforming except for the common nodes. These nodes are referred to as independent since they all match a corresponding pair at the adjacent mesh. Dependent nodes are found at the non-conforming interfaces $\Gamma_\mathrm{I}^{\mathrm{cf}}$ and their nodal solution can be expressed as a function of the solution field at independent nodal points.

The compatibility condition of the solution field $\mathbf{u}$ at the interface Γ_I between two different adjacent domains s and p reads

$$\mathbf{u}^{(s)} = \mathbf{u}^{(p)} \quad \text{at } \Gamma_\mathrm{I}, \tag{2}$$

and is satisfied with the introduction of linear multipoint constraints (LMPC). The set of LMPC is cast in a matrix form using modified Boolean matrices $\bar{\mathbf{B}}^{(s)}$. These matrices are constructed by row-wise concatenation of the tying relations between independent and dependent interface nodes as

$$\left[\begin{array}{ccc} \bar{\mathbf{B}}^{(1)} & \dots & \bar{\mathbf{B}}^{(N_s)} \end{array}\right] = \left[\begin{array}{ccc} \mathbf{B}^{(1)} & \dots & \mathbf{B}^{(N_s)} \\ \mathbf{C}^{(1)} & \dots & \mathbf{C}^{(N_s)} \end{array}\right]. \tag{3}$$

The matrices $\mathbf{B}^{(s)}$ correspond to the standard signed Boolean matrices which account for the compatibility of independent nodes across the interface whereas $\mathbf{C}^{(s)}$ contain the LMPC concerning dependent nodes.

Continuity (2) is accomplished in a dual approach with the introduction of a Lagrange multiplier field. Due to the presence of non-conforming interfaces, a heterogeneous field of Lagrange multipliers

$$\mathbf{\Lambda} = \left[\begin{array}{c} \boldsymbol{\lambda} \\ \boldsymbol{\mu} \end{array}\right] \tag{4}$$

is needed in this approach. The $\boldsymbol{\lambda}$ components account for the independent nodes while $\boldsymbol{\mu}$ represent the forces acting to constrain the dependent nodes.

The resulting system of equations for the decomposed solid Ω can be written as

$$\left[\begin{array}{cccc} \mathbf{K}^{(1)} & \mathbf{0} & \mathbf{0} & \bar{\mathbf{B}}^{(1)\mathrm{T}} \\ \mathbf{0} & \ddots & \mathbf{0} & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{K}^{(N_s)} & \bar{\mathbf{B}}^{(N_s)\mathrm{T}} \\ \bar{\mathbf{B}}^{(1)} & \dots & \bar{\mathbf{B}}^{(N_s)} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{u}^{(1)} \\ \vdots \\ \mathbf{u}^{(N_s)} \\ \mathbf{\Lambda} \end{array}\right] = \left[\begin{array}{c} \mathbf{f}_{\mathrm{ext}}^{(1)} \\ \vdots \\ \mathbf{f}_{\mathrm{ext}}^{(N_s)} \\ \mathbf{0} \end{array}\right], \tag{5}$$

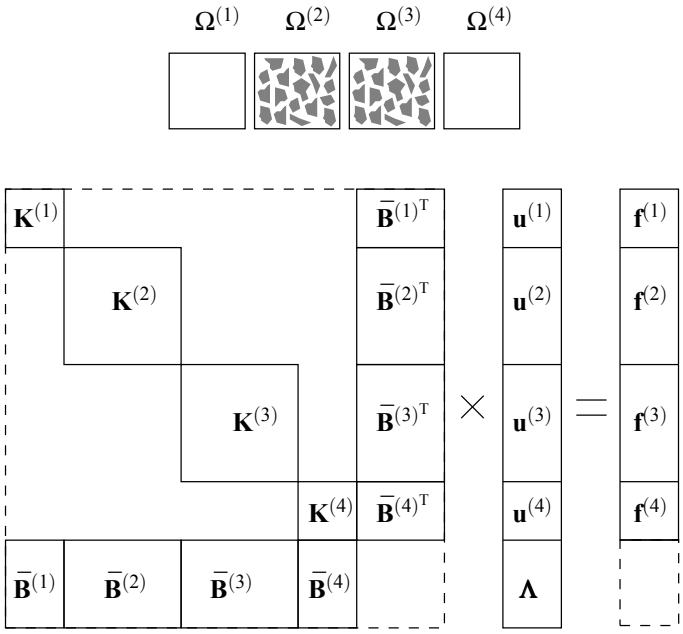

Figure 2: Decomposed structure with different resolutions (top) and corresponding global system of equations arising from a dual connection strategy (bottom).

and is equivalent to the one in (1) when no partitions are considered.

The multiscale analysis of a decomposed structure starts by considering a coarse scale resolution at each domain with homogeneous effective properties. When non-linearities are predicted at domain $\Omega^{(s)}$, the coarse resolution is upgraded to its corresponding fine scale representation which accounts for the lower scale material components. This zoom-in process consists of the solution of a boundary value problem at the fine scale domain and a set of global iterations to satisfy equilibrium [1, 2]. The adaptive nature of the multiscale strategy captures the spread of non-linearity with high resolution discretizations similarly to mesh refinement techniques. For instance, the structure of a system of equations for a body decomposed in four domains with two fine scale resolutions is depicted in Figure 2. Obviously, most of the non-zero entries of the sparse global system are related to fine scale domain quantities such as stiffness and compatibility coefficients.

2.2 Parallel solution strategies

The global system of equations in (5) arising from the multiscale analysis of a heterogeneous structure is inherently large. For this reason, efficient parallel solvers need to be considered. Essentially, the choices reduce to the use of direct and/or iterative solvers.

Direct solvers are based on factorization, e.g. Gaussian factorization, and substitution techniques. They are well known for their robustness but the sequential nature of these algorithms negatively influences the parallel efficiency which deteriorates as the number of processors increases. Iterative solvers, however, are regarded as naturally parallel

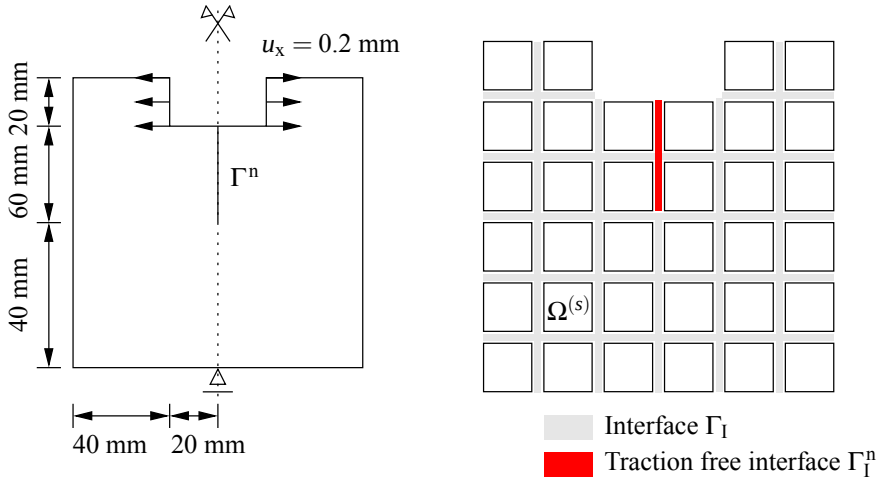

Figure 3: Boundary conditions (left) and domain decomposition (right) for the wedge split test.

strategies since they involve simple operations which are performed in order to simultaneously search for approximations of all unknowns. Unfortunately, their performance can be challenged when accounting for ill-conditioned systems which are often encountered in computational mechanics problems.

An efficient alternative is the use of semi-iterative solvers which rely on domain decomposition of the structure. In these solvers, the augmented system in (5) is transformed, using local factorizations of the domain stiffness $\mathbf{K}^{(s)}$, into an interface problem which is solved iteratively [14]. Although these techniques exhibit good parallel scalability, their performance is linked to the use of efficient preconditioners which is an ongoing research topic for systems arising from highly heterogeneous materials.

Given a reasonable amount of memory, a large sparse system can be tackled with a direct parallel solver using a moderate number of processors. These algorithms are referred to as multi-frontal or block-LU methods and are based on independent simultaneous factorizations of the domain matrices. Although these techniques do not scale well in massively parallel computers, they provide the same robustness as traditional direct methods which make them attractive when dealing with ill-conditioned systems. In our examples a direct parallel solver which takes into account automatic load-balancing and multi-threading is utilized for the solution of the global system in (5).

3 MULTISCALE ANALYSIS OF A WEDGE SPLIT TEST

The multiscale analysis of the wedge split test, presented in [15], is sketched in Figure 3 and is reproduced in this contribution to prove the objectivity of the multiscale framework. The material sample is decomposed into a number of non-overlapping domains and the notch Γ^n is modelled by means of the traction free interface Γ_I^n. A concrete-like material with three phases (aggregate, matrix and an interface transition zone) is considered in the

	Material parameters		Aggregates	Matrix	ITZ
E	Young's mod.	[GPa]	35.0	30.0	20.0
ν	Poisson's ratio	[-]	0.2	0.2	0.2
$\tilde{\varepsilon}_{nl}$	Non-loc. equiv. strain	[-]	Mazars	Mazars	Mazars
κ_0	Dam. init. thres.	[-]	dummy	0.124×10^{-4}	0.1×10^{-4}
c	Grad. param.	[mm^2]	0.75	0.75	0.75
$\omega(\kappa)$	Dam. evol. law	[-]	Exp.	Exp.	Exp.
α	Resid. stress param.	[-]	0.999	0.999	0.999
β	Soft. rate param.	[-]	500	500	500
	Two-dimensional analysis type			Plane strain	

Table 1: Material data for the concrete specimen.

fine scale discretization. The coarse discretization consists of a homogeneous bulk with effective elastic properties. A gradient-enhanced damage model [16] is adopted and the material parameters for each phase are listed in Table 2. The selected micro-to-macro connection enforces an equivalent coarse and fine solution field at the interfaces $\Gamma_{\mathrm{I}}^{\mathrm{cf}}$ and is referred to as full collocation technique in [2].

3.1 Objectivity analysis

The proposed multiscale approach requires the input of three main variables or parameters that are crucial for a complete set up of the analysis. These parameters need to be defined by the user and are identified as:

- the fine scale discretization used to describe all mesoscopic heterogeneities,
- the coarse scale discretization used at the homogeneous linear elastic bulk, and
- the domain decomposition (size and geometry of the mesh partitions).

Consequently, the result of the adaptive multiscale analysis needs to be completely independent of the three user-defined parameters.

Objectivity with respect to the fine scale discretization is trivial to justify provided that a regularized model is utilized to simulate the envisaged material non-linearity. Mesh independent results are automatically guaranteed by the gradient-enhanced damage model given a minimum size of the FEs which is connected to the gradient parameter c.

The size of the coarse scale FEs need to be sufficiently small in order to correctly reproduce the spatial variation of the solution field gradients during the linear elastic regime. To this end, error estimators should be utilized to ensure that the coarse scale discretization is fine enough throughout the elastic regime. This feature is not accounted for in the present study since it is assumed that the coarse scale discretization provided at the initial stage is already appropriate. Nevertheless, a sensitivity analysis is performed on the wedge split example in which three different coarse meshes are selected.

The wedge split test, considering a decomposition into 34 domains, is reproduced for an initial coarse discretization of 2176, 8704 and 34816 bilinear Q4 elements at the whole sample, i.e. including all domains. As shown in Figure 4 (left) the damage contours are plotted for the last loading stage. No significant differences can be observed between damage plots. The resulting force-displacement responses turn out to be in good agreement with the DNS, i.e. considering all fine discretizations from the start. In Figure 5 the maximum relative error between multiscale analyses and the DNS at the peak is around 0.02%. This value corresponds to the coarsest discretization (2176 Q4) and the error diminishes upon mesh refinement. Consequently, the response of the multiscale framework is objective with respect to the coarse scale mesh.

The wedge split test is again reproduced considering the intermediate coarse discretization (8704 Q4) and three domain decompositions with 34, 68 and 136 partitions. Now the discretization of the coarse scale and fine scale is fixed. No remarkable differences can be noticed by visual inspection of the damage distribution plots in Figure 4 (right). This indicates that the decomposition does not influence material non-linearity in the sample and, therefore, the overall mechanical response is not changed. By inspecting the resulting force-displacement response in Figure 6 the maximum relative error between multiscale analyses and the DNS at the peak is around 0.06%. The highest overestimation of the peak load corresponds to the partition into 136 domains. This can be explained considering that a lower fine scale area is accounted for in this analysis and, therefore, the solution is slightly stiffer due to the larger amount of coarse scale domains. Essentially, it can be concluded that the response of the multiscale framework is objective with respect to the domain decomposition.

3.2 Parallel performance

The global assembled system is solved using a parallel solver designed for the solution of large sparse linear systems based on direct methods [17]. Automatic load-balancing and multi-threading are accounted for and, consequently, the performance of the solver is optimized according to the hardware used.

All analyses have been performed on a Dell R710 PowerEdge machine: 2 X5570 quad-core Xeons (Core I7 Nehalem) clocked at 2.93 GHz with 24 GB of memory. Parallel tasks related to BVP solves of different zoomed-in domains and FE assemblies are distributed over the four cores using message passing interface. The direct parallel solver [17] is utilized for the solution of the global system (5) with the available four cores.

There are approximately one million degrees of freedom involved in the DNS and the complete analysis is carried out using 200 loading steps. The total number of Newton-Raphson (NR) iterations needed to complete the DNS is 686 and the analysis is finished after 16409 seconds. The adaptive nature of the multiscale analyses provides a faster solution which oscillates between 61% and 88% of the total DNS time (see Table 3.2).

The size of the multiscale problem is proportional to the spread of non-linearity. The non-linear region is efficiently covered when a high number of small domains is considered

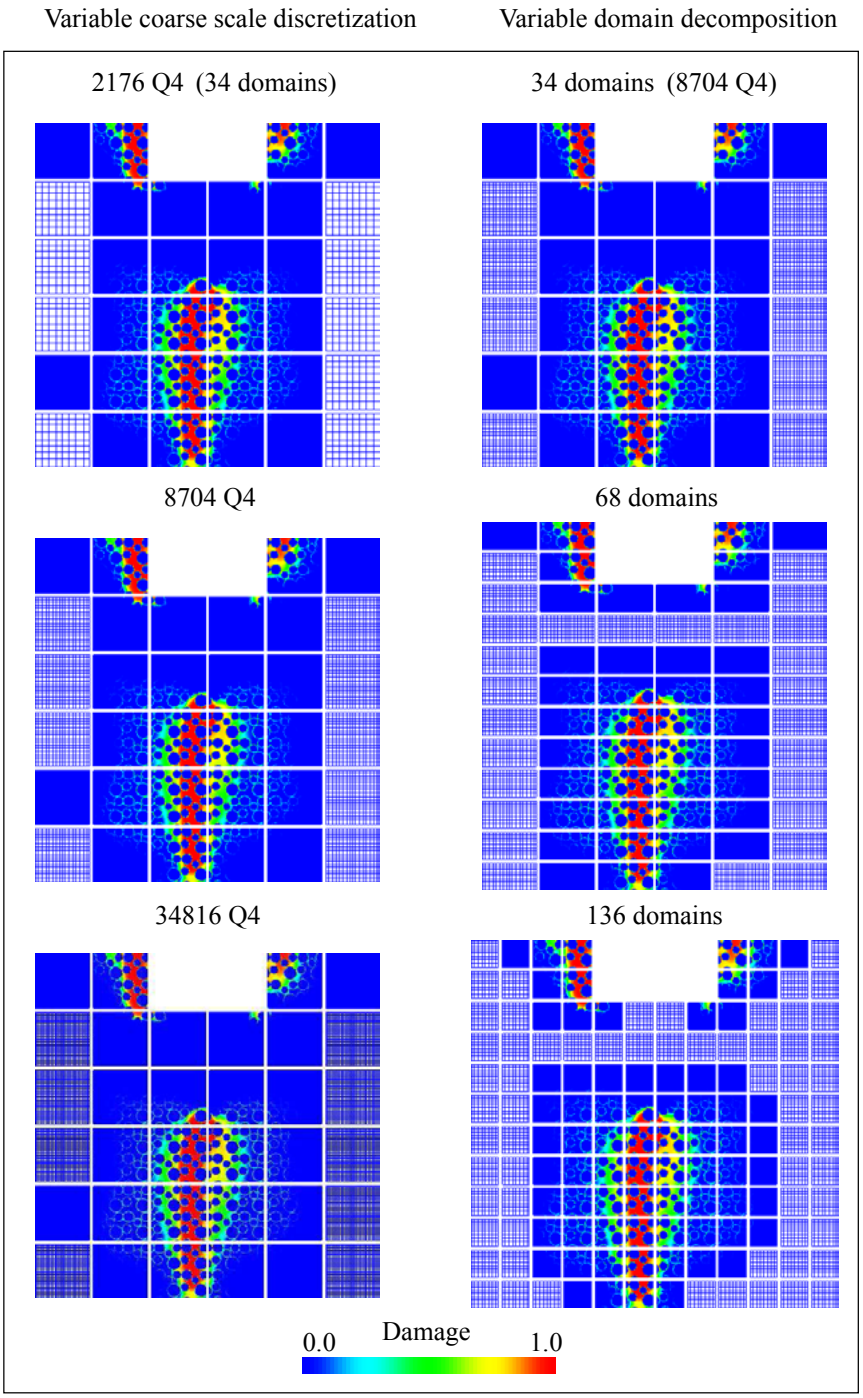

Figure 4: Damage distribution at ultimate loading stage with different coarse discretizations (left) and domain decompositions (right). Results are shown in the undeformed meshes.

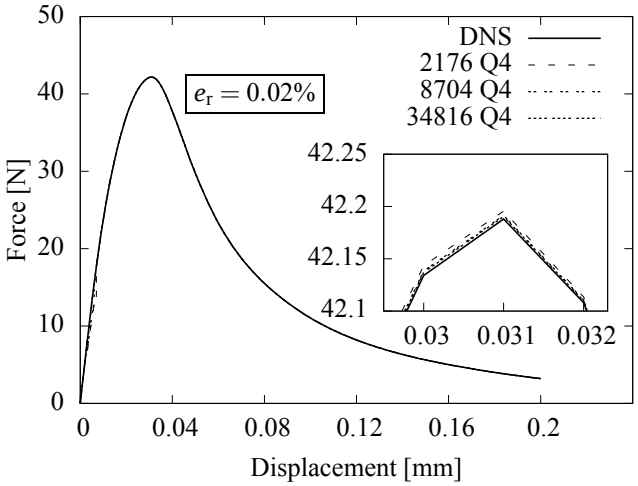

Figure 5: Force-displacement plots for different coarse discretizations and a decomposition in 34 domains.

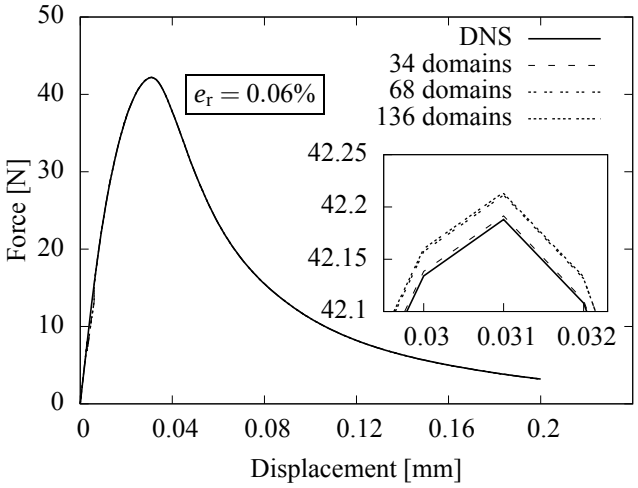

Figure 6: Force-displacement plots for different domain decompositions and a coarse discretization of 8704 Q4 elements.

Analysis	Zoom-in steps	NR iterations	Final zoom-in ratio (%)	Solve time (seconds)
DNS	-	686	-	16409
34 domains	14	821	74	14395
68 domains	18	853	60	10063
136 domains	32	960	53	11577

Table 2: Material data for the concrete specimen.

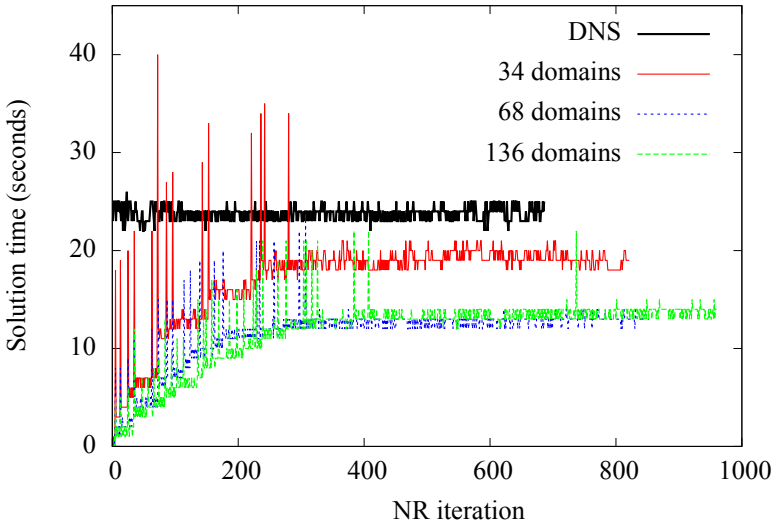

Figure 7: Total solution time at each NR iteration.

and, for this reason, these analyses tend to provide lower solution times. However, the number of zoom-in stages clearly slows down the solution process. Each zoom-in stage is registered as a peak in the total solution time evolution in Figure 7. This is due to the computation of the BVP and re-calculation of the connectivity matrices $\bar{\mathbf{B}}^{(s)}$.

Another competing effect is the proportion between stiffness coefficients and connectivity coefficients in the global system. This is specially visible at the total solution times corresponding to the last iterations using 68 and 136 domains (Figure 7). All zoom-in stages have been performed at this part of the analysis and the solution time per iteration for when using 136 domains is slightly higher than the one employing 68 domains. The off-diagonal terms related to the matrices $\bar{\mathbf{B}}^{(s)}$ induce a more laborious solving procedure which diminishes the performance of the computations.

4 CONCLUSIONS

The concurrent multiscale framework selected in this contribution is assessed for the study of heterogeneous quasi-brittle materials which show localized failure patterns. The results of the concurrent multiscale framework turn out to be in good agreement with DNS and objectivity of the analyses with respect to user-defined parameters, i.e. initial coarse scale discretization and domain decomposition, is observed.

The efficiency of the presented approach is still moderate in our academical analyses but increases when the spread of non-linearity is significantly low compared to the size of the structure. This is the case of large structures with high stress concentrations due to localized loads, irregular geometries or non-uniform distribution of the mesoscopic structure.

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