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High-Performance Mechanically Regularized Finite-Element Digital Volume Correlation for Complex Architected Materials

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Abstract — Measuring kinematic fields at the architecture scale of cellular materials is known to be highly challenging in experimental mechanics, in particular because of the geometric complexity of the specimen and the poor texture at this scale. To overcome this obstacle, a solution consists in assisting Digital Volume Correlation (DVC) with a FE-based mechanical regularization. However, such approaches entail a substantial computational burden when considering complex architected materials along with large volume images. To address this issue, this study proposes a scalable domain decomposition algorithm to efficiently estimate subcellular kinematic fields across large regions of cellular materials.

Keywords — DVC, HPC, Mechanical Regularization, Domain Decomposition, Parallel computing

Introduction Architected materials are excellent candidates for the design of multifunctional structures with outstanding specific properties. However, due to the coexistence of two very different scales, the prediction of the mechanical behavior of such materials remains an issue. This is especially true for synthetic materials such as foams because of their random architecture. Their mechanical characterization requires conducting *in-situ* experiments on real and representative cellular material samples. In this context, X-ray Computed Tomography (CT) scans provide a three-dimensional insight into specimens, which enables the analyses of such structures at different loading stages. Then, Digital Volume Correlation (DVC) enables the quantitative analysis of these series of volume images and the consequent extraction of relevant displacement fields.

These volume images contain a huge amount of data, enabling detailed observation of the geometric complexity of cellular material architecture. Yet, the inherent texture of the material at this scale is too poor to measure subcellular kinematic fields with DVC. To overcome this obstacle, a solution consists in considering FE-based DVC and complementing it with a finely-tuned mechanical regularization [1] to assist the correlation below the cell scale. However, such FE-DVC approaches come with a high numerical complexity compared to subset-DVC, as the former entail solving multiple (sparse but) global linear systems, while the latter involve smaller and independent systems of equations formulated on each subset which are parallelizable. Hence, numerous CPU and GPU parallel computing techniques have been employed to accelerate subset DVC methods due to their inherent parallel nature [2]. Much less work has been done on the parallelization of FE-DVC (using GPU for instance in [3, 4]).

This work focuses on developing and implementing a scalable algorithm for solving a mechanically regularized FE-DVC problem using domain decomposition [5] to parallelize the solution.

Methods The DVC problem is based on the gray level conservation equation. The displacement field is discretized using a FE mesh of the architecture of the specimen built on the image (see [1] for more details). To simplify the formulation of the domain decomposition method, we consider the mechanical regularization based on the potential FE energy as introduced in [6]:

$$\mathbf{u}^* = \arg \min \phi_{cor}(\mathbf{u}) + \alpha \left(\frac{1}{2} \mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{u}^T \bar{\mathbf{f}} \right),$$

where ϕ_{cor} represents the classical DVC functional, \mathbf{K} the FE stiffness matrix and $\bar{\mathbf{f}}$ an approximation of distribution forces at the boundaries. This force distribution is calculated based on an *a priori* assumption

about the displacement field, which is obtained by initially solving the DVC problem with standard Tikhonov regularization.

The Cartesian partitioning employed for domain decomposition produces conforming and non-overlapping submeshes. To ensure that the submesh locally deformed by the computed solution \mathbf{u}^* remains fully contained within its corresponding subimage, we introduced a slight overlap in the volume image partitioning. The algorithm was constructed in 3 steps and implemented in Python for parallel solution with distributed memory. PETSc (`petsc4py`) is used for iterative and direct solving and domain decomposition management [7]. The first solution is computed in parallel with local solve on each subdomain. This step serves as an initialization for a global parallel solution with standard Tikhonov regularization. The obtained result initializes the distribution forces $\bar{\mathbf{f}}$ used for the mechanical regularization and then solves the global problem.

Results The proposed algorithm is used to solve the problem on $(827 \times 757 \times 761)$ voxels 8-bit 3D CT scans of an *in-situ* compression of a polyurethane foam cylinder (see, again, [1]). The tested sample has a diameter of 9 mm and a height of 10 mm. The considered stage of loading corresponds to a 3.4 %-overall strain in order. The voxel size is about $13.34 \mu\text{m}$. The mesh, shown on figure 1a, has 2 976 000 nodes and 8 928 009 elements. The average element size is 2.6 voxels. The convergence of a solution towards a displacement field at architecture scale and under little texture is demonstrated on figure 1b. The strong scalability of the proposed algorithm is illustrated on figure 1c. The sequential resolution on ISAE-Supaero cluster takes 34 min 25 s whereas the resolution with 32 processors takes 1 min 20 s.

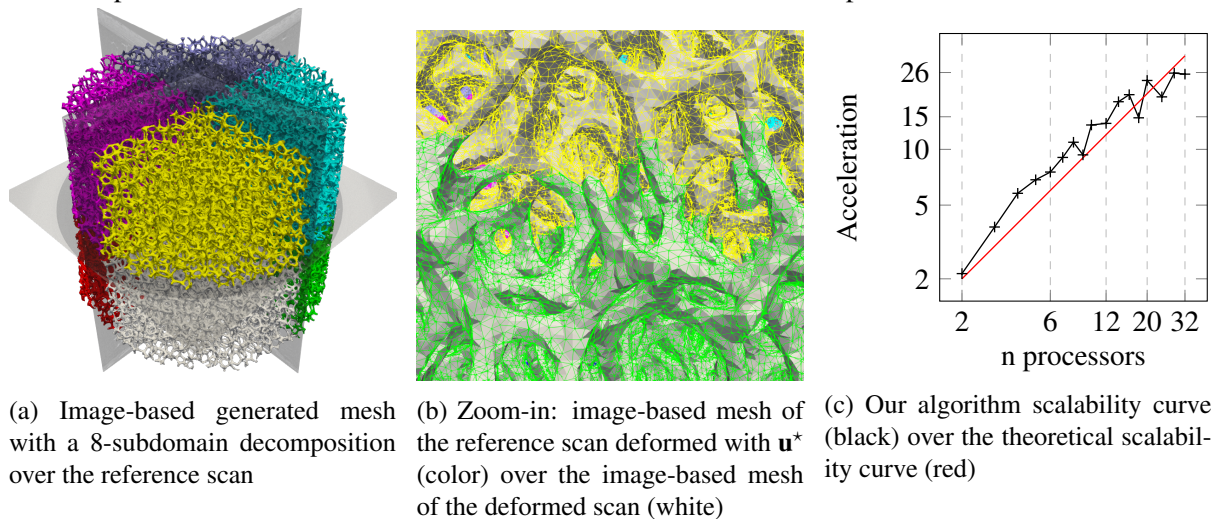


Figure 1: Mechanical and computational results of the proposed algorithm on a polyurethane foam.

Conclusion This study proposed a domain decomposition mechanically regularized FE-DVC algorithm for a parallel solution with distributed memory. The strong scalability of the implemented algorithm is demonstrated, opening the door for addressing highly complex applications starting by analyzing the other scans at higher deformation levels.

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